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Addendum to :

'Crystallographic Computing at Oak Ridge National Laboratory: 1954 to 1968' by William Busing; and other articles

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Addendum Table of Contents

(This issue's editor: Lachlan Cranswick)

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A crystallographic least squares refinement program for the IBM 704, ORNL-CF-59-4-37, Oak Ridge, TN : Oak Ridge National Laboratory, 1959. 2
W. R. Busing and H. A. Levy

A crystallographic function and error program for the IBM 704, ORNL-CF-59-12-3, Oak Ridge, TN : Oak Ridge National Laboratory, 1959. 148
W. R. Busing and H. A. Levy

OR ABS : a FORTRAN program for calculating single crystal absorption corrections, ORNL-TM-229, Oak Ridge, TN : Oak Ridge National Laboratory, 1962. 246
D. J. Wehe, W. R. Busing and H. A. Levy

OR GLS : a general fortran least squares program, ORNL-TM-271, Oak Ridge, TN : Oak Ridge National Laboratory, 1962. 294
W. R. Busing and H. A. Levy

OR FLS, A Fortran crystallographic least-squares program, ORNL-TM-305, Oak Ridge, TN : Oak Ridge National Laboratory, 1962. 340
W. R. Busing, K. O. Martin, and H. A. Levy

OR FFE, a FORTRAN crystallographic function and error program, ORNL-TM-306, Oak Ridge, TN : Oak Ridge National Laboratory, 1964. 424
W. R. Busing, K. O. Martin, and H. A. Levy

OR TEP : A Fortran thermal-ellipsoid plot program for crystal structure illustrations, ORNL-3794, Oak Ridge, TN : Oak Ridge National Laboratory, 1965. 516
Carroll K. Johnson

OR TEP-II : a FORTRAN Thermal-Ellipsoid Plot Program for crystal structure illustration, ORNL-5138, Oak Ridge, TN : Oak Ridge National Laboratory, 1976. 650
Carroll K. Johnson

Reprint courtesy of Oak Ridge National Laboratory, Tennessee, USA:

A crystallographic least squares refinement program for the IBM 704, ORNL-CF-59-4-37, Oak Ridge, TN : Oak Ridge National Laboratory, 1959

by W. R. Busing and H. A. Levy

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A CRYSTALLOGRAPHIC LEAST SQUARES REFINEMENT PROGRAM FOR THE IBM 704

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A CRYSTALLOGRAPHIC LEAST SQUARES REFINEMENT PROGRAM FOR THE IBM 704

By

William R. Busing and Henri A. Levy
Chemistry Division, Oak Ridge National Laboratory
Oak Ridge, Tennessee

April, 1959

IDENTIFICATION

Symbolic decks OR XLS, OR XLS 1, 2, 3, 4, 5, 6.

Binary decks OR XLS A, B, C, D, E, F, G, H, J, K, L, M, N.

DATE ISSUED

MAY - 4 1959

ERRATA FOR CF 59-4-37

September 22, 1959

Page 57

```
01364  0 00000 0 00077  IFF11 PZE 63          MASK
```

Page 63

```
00624  0 76100 0 00000         NOP
00625  0 76100 0 00000         NOP
00626  0 76100 0 00000         NOP
```

Page 114

```
05133  0 00000 0 00077  IFF11 PZE 63          MASK
```

Page 134

```
00126  0 76200 0 00225  MB     RTB 5
00127  0 76200 0 00225         RTB 5
00130  0 50000 0 01314  MC     CLA N
00131 -0 10000 0 00142         TNZ ME

00143  0 76200 0 00225         RTB 5
00144  0 76200 0 00225  ME3    RTB 5
00145  0 70000 0 01315         CPY A
00146  0 02000 0 00144         TRA ME3
```

WRB:vj
9/22/59

CHANGES FOR CF 59-4-37

November 30, 1959

The following changes and additions should be made in ORNL CF 59-4-37 to make it consistent with the binary change cards dated November 30, 1959:

Page 44

```
00151  0 02000 0 00353          TRA KA
00156  0 02000 0 00355          TRA KF
```

Page 46

```
00271  0 07400 4 00241  KA1     TSX RTB,4
```

Page 47

```
00337  0 76200 0 00225  KF4     RTB U3

00353  0 77200 0 00204  KA      REW U1
00354  0 02000 0 00271          TRA KA1
00355  0 77200 0 00205  KF      REW U3
00356  0 76200 0 00225          RTB U3
00357  0 76200 0 00225          RTB U3
00360  0 76200 0 00225          RTB U3
00361  0 02000 0 00337          TRA KF4
```

WRB:vj
12/2/59

ORNL 59-4-37

A CRYSTALLOGRAPHIC LEAST SQUARES PROGRAM FOR THE IBM 704

ADDENDA AND ERRATA

June 7, 1960

Addendum

Page 19, after line 14 from bottom.

Stops at 3513 (8) or 3672 (8) in OR XLS2 indicate that the matrix is essentially singular but in a way not detected by the matrix inverter.

Program Changes

Binary correction cards for these changes were distributed on June 6, 1960.

Page 124, line 31

```
00506   0  62200 0 00552        STD XJL
```

Page 125, lines 24-31

```
00552  -3  00000 4 00570  XJL   TXL XJS,4,0 DECREMENT TO
                                            BE SET
00553   0  70000 4 00000        CPY 0,4
00554   0  02000 0 00557        TRA XJM
00555   0  00000 0 00000        PZE
00556   0  02000 0 00573        TRA XJT
00557  -0  76000 0 00001  XJM   PBT
00560   0  02000 0 00562        TRA XJO
00561   1  77777 4 00562  XJN   TXI XJO,4,-1
```

Errata

Page 59, line 2 from bottom.

```
03171   0  00000 0 00000  T5    4(SIN THETA/LAMBDA)**2
```

Page 60, line 1.

```
03173   0  00000 0 00000  T7    CURRENT VALUE OF Q. SEE M6
```

Page 60, lines 15 and 16.

```
03223   0  00000 0 00000  M6    Q, SCALE FACTOR DESIGNATION
03224   0  00000 0 00000  M7    (SIN THETA/LAMBDA)**2=RHO
```

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GENERAL DESCRIPTION

OR XLS1-5 is a program for structure factor calculation and for the least squares refinement of crystal structures using X-ray or neutron diffraction data. The code is divided into five segments and the purpose of each will be described briefly:

OR XLS1 is the preliminary data processing segment. Its input data include the reciprocal cell parameters, the form factor tables (unless problem is a neutron one), and the data for each observation. The latter consist of the indices, the observed structure factor or its square, the estimated standard error of the observation, and an indication of which of several scale factors is to be applied. The output of this segment consists of a binary tape with the input data together with $(\sin \theta/\lambda)^2$ and the interpolated form factors for each reflection. The same information may also be put out in BCD form for off-line printing.

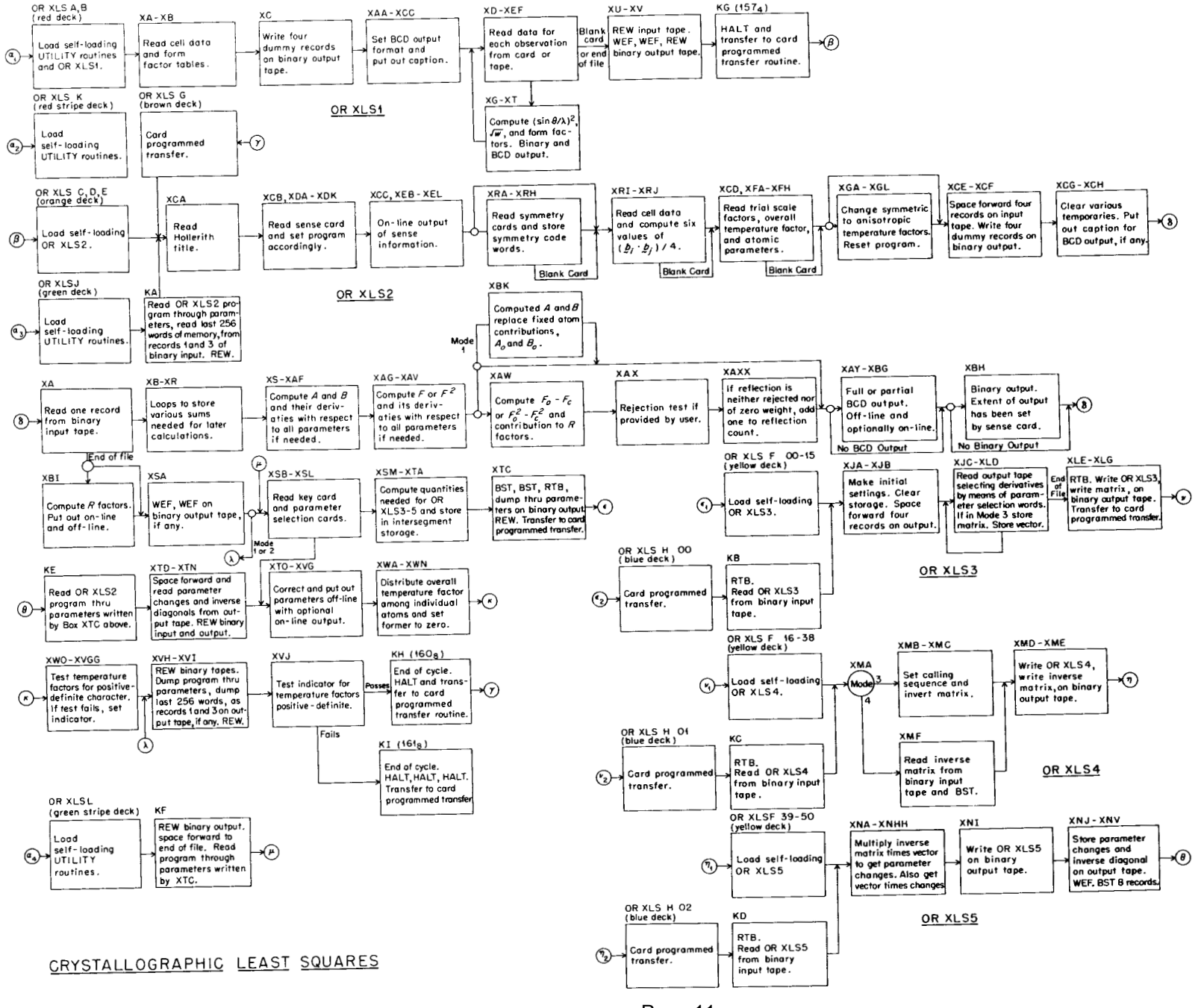
OR XLS2 is the main segment for least squares and structure factor calculations. Its input data consist of a sense card which specifies several options available to the user, symmetry information, reciprocal cell data, and trial parameters including an arbitrary number of scale factors, overall temperature factor coefficient, and, for each atom, the position parameters and one or six temperature factor coefficients. Also used as input is the binary tape from OR XLS1. The primary output of this segment when it is used for least squares is a binary tape on which are stored the derivatives of F_c or F_c^2 with respect to the parameters for each observation. The calculated structure factors may also be put out during this part of the calculation.

For a structure factor calculation this completes the problem. For least squares OR XLS2 calls for the input of parameter selection cards which specify the parameters to be adjusted. OR XLS3 then uses the derivatives from the binary output tape to set up the matrix and vector of the normal equations. OR XLS4 inverts this matrix, and OR XLS5 multiplies the resulting inverse by the vector to obtain the parameter changes.

Control is then returned to OR XLS2 which adjusts the parameters and puts them out off-line and optionally on-line.

During each cycle the input data for each reflection is copied onto the binary output tape as are the programs and input data for OR XLS2-5 so that this tape may serve as the main input for the next cycle.

An optional output of the matrix of the normal equations or its inverse is provided.



CRYSTALLOGRAPHIC LEAST SQUARES

MACHINE REQUIREMENTS

Minimum 704 with

1. 8192 word core storage or more
2. 3 on-line tape units
3. CAD instruction
4. Off-line tape printer.

CAPACITY

Core storage	Maximum number of parameters varied simultaneously
8,192	120
16,384	175
32,768	251

MATHEMATICAL METHOD

In this section the details of the computation will be briefly outlined.

OR XLS1

For each reflection this segment computes

$$\rho = (\sin\theta/\lambda)^2 = (.25)(h^2a^{*2} + k^2b^{*2} + \ell^2c^{*2} + 2hka^*b^*\cos\gamma^* + 2h\ell a^*c^*\cos\beta^* + 2k\ell b^*c^*\cos\alpha^*)$$

where a^*, b^*, c^*, $\cos\alpha^*$, $\cos\beta^*$, and $\cos\gamma^*$ are the reciprocal cell constants and h, k, and ℓ are the indices of the reflection.

Also computed for each reflection is $\sqrt{w} = 1/\sigma$ where σ is the standard error of the observed $|F|$ or F^2, whichever is being refined, and w is the least squares weight of the observation. (If $\sigma = 0$ the program sets $\sqrt{w} = 0$.)

For X-ray problems the atomic form factors for each observation are obtained by linear interpolation in the form factor tables which are stored at intervals of 0.05 in $\sin\theta/\lambda$.

The fixed atom contributions, A_o and B_o, (see below) are set at zero.

OR XLS2

Included in the data for this segment are the r scale factors s_q, overall temperature factor coefficient T_o, and the individual atom parameters. The latter are f_i, x_i, y_i, z_i, and T_i if symmetric temperature factors are to be used or f_i, x_i, y_i, z_i, β_{11i}, β_{22i}, β_{33i}, β_{12i}, β_{13i}, and β_{23i} for anisotropic temperature factors. For X-ray work f_i is an integer which indicates which form factor is to be used, while for neutron work it is the scattering factor itself.

If the sense card indicates that symmetric temperature factors are to be converted to anisotropic form the routine computes for each atom

$$\beta_{11i} = T_i a^{*2}/4$$
$$\beta_{12i} = T_i a^* b^* \cos\gamma^*/4$$
$$\text{etc.,}$$

relocates the parameters in anisotropic form, and resets the program on this basis.

The expressions for the scaled structure factor or its square and the derivatives of these with respect to the parameters are summarized in the following table:

	Centrosymmetric with origin at symmetry center	Acentric
(s_qF)	$2s_q \exp(-T_o\rho)A$	$s_q \exp(-T_o\rho)(A^2 + B^2)^{1/2}$
$\partial(s_qF)/\partial s_q$	$(s_qF)/s_q$	$(s_qF)/s_q$
$\partial(s_qF)/\partial T_o$	$-\rho(s_qF)$	$-\rho(s_qF)$
$\partial(s_qF)/\partial p$	$2s_q \exp(-T_o\rho)(\partial A/\partial p)$	$s_q \exp(-T_o\rho)(A^2 + B^2)^{-1/2}\left[A(\partial A/\partial p) + B(\partial B/\partial p)\right]$
$(s_qF)^2$	$4s_q^2 \exp(-2T_o\rho)A^2$	$s_q^2 \exp(-2T_o\rho)(A^2 + B^2)$
$\partial(s_qF)^2/\partial s_q$	$2(s_qF)^2/s_q$	$2(s_qF)^2/s_q$
$\partial(s_qF)^2/\partial T_o$	$-2\rho(s_qF)^2$	$-2\rho(s_qF)^2$
$\partial(s_qF)^2/\partial p$	$8s_q^2 \exp(-2T_o\rho)A(\partial A/\partial p)$	$2s_q^2 \exp(-2T_o\rho)\left[A(\partial A/\partial p) + B(\partial B/\partial p)\right]$

Here F is the structure factor, s_q is the scale factor, T_o is the overall temperature factor coefficient, ρ is $\sin^2\theta/\lambda^2$, A and B are the real and imaginary components of the structure factor, and p is any individual atom parameter.

The expressions for A and B and their derivatives are summarized as follows:

	Symmetric temperature factor	Anisotropic temperature factor
A	$A_o + \sum_i f_i \exp(-T_i\rho) \sum_j \cos_{ij}$	$A_o + \sum_i f_i \sum_j \exp_{ij}\cos_{ij}$
B	$B_o + \sum_i f_i \exp(-T_i\rho) \sum_j \sin_{ij}$	$B_o + \sum_i f_i \sum_j \exp_{ij}\sin_{ij}$
$\partial A/\partial f_i$	$\exp(-T_i\rho) \sum_j \cos_{ij}$	$\sum_j \exp_{ij}\cos_{ij}$
$\partial B/\partial f_i$	$\exp(-T_i\rho) \sum_j \sin_{ij}$	$\sum_j \exp_{ij} \sin_{ij}$

	Symmetric temperature factor	Anisotropic temperature factor
$\partial A/\partial T_i$	$-\rho f_i \exp(-T_i\rho) \sum_j \cos_{ij}$	-----
$\partial B/\partial T_i$	$-\rho f_i \exp(-T_i\rho) \sum_j \sin_{ij}$	-----
$\partial A/\partial x_i$	$-2\pi f_i \exp(-T_i\rho) \sum_j h'_j \sin_{ij}$	$-2\pi f_i \sum_j h'_j \exp_{ij} \sin_{ij}$
$\partial B/\partial x_i$	$2\pi f_i \exp(-T_i\rho) \sum_j h'_j \cos_{ij}$	$2\pi f_i \sum_j h'_j \exp_{ij} \cos_{ij}$
$\partial A/\partial \beta_{12i}$	-----	$-f_i \sum_j (2hk)'_j \exp_{ij} \cos_{ij}$
$\partial B/\partial \beta_{12i}$	-----	$-f_i \sum_j (2hk)'_j \exp_{ij} \sin_{ij}$

Here the subscripts i and j refer to the various atoms in the asymmetric unit and to the different equivalent positions, respectively. The terms $\cos_{ij}$, $\sin_{ij}$, and $\exp_{ij}$ are the trigonometric contributions and the anisotropic temperature factor of atom i in equivalent position j. The expressions h'_j and $(2hk)'_j$ are representative of the transformed indices and index products. All of these terms are discussed in detail in the section on Symmetry Considerations.

T_i and f_i are the symmetric temperature factor coefficient and scattering factor, respectively, of atom i. A_o and B_o are the contributions to A and B of fixed atoms, i.e., atoms not represented in the parameter table, and which are therefore not to be adjusted by the least squares procedure. For each reflection these terms are taken from the binary input tape, and they will be zero unless they have been computed using mode 1. Mode 1 is in every way similar to a structure factor calculation except that initially A_o and B_o are set to zero and finally they are set to equal to computed A and B. These computed values are then copied from tape to tape during the various least squares or structure factor computations until they are replaced by a new mode 1 calculation.

The program does the computation for each reflection in three steps. First the sums over j are accumulated. These are then converted to the derivatives of A and B with respect to the atomic parameters, and A and B are obtained. Finally the scaled structure factor or its square and the derivatives of this quantity

are computed. In determining which expressions to evaluate the program considers whether derivatives are needed or not, whether centrosymmetric or acentric computation is specified on the sense card, and whether the temperature factors are symmetric or anisotropic. Note that, except for the above restrictions, the program evaluates and stores on the binary output tape derivatives with respect to all the parameters regardless of which ones are to be varied.

A mode of operation (mode 4) is available in which the derivatives are not computed but rather are copied from the input tape where they were stored on a previous cycle. It is possible that this mode of operation will permit the running of several cycles in a minimum amount of time.

The following table gives the expressions for Δ, the difference between the observed and calculated structure factors or their squares, and for the various discrepancy factors which are computed while the structure factors and derivatives are being obtained.

	Refining of F	Refining on F^2
Δ	$\left[(\text{sign of } s_qF)\lvert F_o\rvert\right] - s_qF$	$F_o^2 - (s_qF)^2$
R	$\sum\lvert\Delta\rvert \Big/ \sum\lvert F_o\rvert$	$\sum\lvert\Delta\rvert \Big/ \sum\lvert F_o^2\rvert$
Weighted R	$\sqrt{\sum(\sqrt{w}\,\Delta)^2} \Big/ \sqrt{\sum(\sqrt{w}\,F_o)^2}$	$\sqrt{\sum(\sqrt{w}\,\Delta)^2} \Big/ \sqrt{\sum(\sqrt{w}\,F_o^2)^2}$
Error of fit	$\sqrt{\sum(\sqrt{w}\,\Delta)^2} \Big/ \sqrt{(m-n)}$	$\sqrt{\sum(\sqrt{w}\,\Delta)^2} \Big/ \sqrt{(m-n)}$

For the two R factors the summations are made both over all observations and over all non-zero observations. For the error of fit the summation is made over all reflections used in the least squares refinement, i.e., those with non-zero weight which pass the rejection test (if such a test is supplied by the user). The number of such observations is m and the number of parameters adjusted is n. (Before any refinement has been performed the program considers that n = 0.) These discrepancy factors refer, of course, to the input parameters.

Δ and $\sqrt{w}\,\Delta$ are put out with the structure factors under the headings OBS-CALC and (OBS-CALC)/SIGMA, respectively. Reflections for which the latter is greater than 2 (the constant stored at C7) are marked with a double asterisk (**).

OR XLS3

The function of this segment is to store the matrix $\underset{\sim}{a}$ and the vector $\underset{\sim}{v}$ of the normal equations. The elements of these are

$$a_{ij} = \sum (\sqrt{w}\, D_i)(\sqrt{w}\, D_j)$$

$$v_i = \sum (\sqrt{w}\, D_i)(\sqrt{w}\, \Delta)$$

where the summations are over the un-rejected observations of non-zero weight. For each reflection the n derivatives, D_i, are selected from the binary output tape and correspond to those parameters which are to be adjusted.

When operating in mode 4 only the vector $\underset{\sim}{v}$ is computed.

OR XLS4

This segment produces the inverse matrix $\underset{\sim}{b} = \underset{\sim}{a}^{-1}$ by a method to be described elsewhere (SHARE ROUTINE OR-SMI).

When mode 4 is specified the program copies the inverse matrix of the previous cycle from the binary input tape instead of inverting the matrix. In either case the resulting inverse is copied onto the binary output tape for use in the next cycle if needed.

OR XLS5

In this segment the parameter changes $\Delta p_i = \sum_j b_{ij} v_j$ are computed and stored on the binary output tape along with the diagonal elements b_{ii} of the inverse matrix. Also computed is $\sum_i \Delta p_i v_i$, the estimated decrease of $\sum (\sqrt{w}\, \Delta)^2$ produced by these parameter changes.

OR XLS2

Control is then returned to this segment and an estimated new value of the standard error of fit,

$$\sqrt{\left[\sum (\sqrt{w}\, \Delta)^2 - \sum_i \Delta p_i v_i \right]} \Big/ \sqrt{(m-n)},$$

is computed. The parameters p_i are corrected by Δp_i and their standard errors computed as

$$\sigma(p_i) = \sqrt{b_{ii}} \sqrt{\left[\sum (\sqrt{w}\, \Delta)^2 - \sum_i \Delta p_i v_i \right]}.$$

At this point the program puts out the old and new parameters with the parameter changes and standard errors for those which have been adjusted.

If the overall temperature factor T_o is not zero the program now adds it to the individual atom temperature factors so that $T_i' = T_i + T_o$ for symmetric temperature factors or

$$\beta_{11}' = \beta_{11} + T_o\, a^{*2}/4$$
$$\beta_{12}' = \beta_{12} + T_o\, a^* b^* \cos\gamma^*/4$$
$$\text{etc.}$$

for anisotropic temperature factors. T_o is then set to zero. These operations are performed so that the temperature factor coefficients may be tested for positive definite character as described below. Note that the result is not strictly correct if fixed atom contributions are used so that it is probably desirable to hold T_o at zero in this case.

The temperature factor coefficients are then tested to insure that the following conditions hold. For symmetric temperature factors:

$$T_i \geq +0.$$

For anisotropic temperature factors:

$$\beta_{11} \geq +0,\ \beta_{22} \geq +0,\ \beta_{33} \geq +0,$$
$$\begin{vmatrix} \beta_{22} & \beta_{23} \\ \beta_{23} & \beta_{33} \end{vmatrix} \geq +0, \quad \begin{vmatrix} \beta_{11} & \beta_{13} \\ \beta_{13} & \beta_{33} \end{vmatrix} \geq +0, \quad \begin{vmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{vmatrix} \geq +0,$$
$$\begin{vmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & \beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{vmatrix} \geq +0.$$

Failure of one of these tests means that the coefficients do not represent physical reality. The use of these parameters in subsequent calculations may cause a programmed stop indicating a negative argument for the temperature factor. When a test fails the program prints out an indication of this failure, and at the end of the calculation the programmed stop is at KI rather than at KH.

SYMMETRY CONSIDERATIONS

General positions

OR XLS2 computes structure factors or their squares in one of the following ways:

$$\left.\begin{aligned} s_qF &= 2s_q\exp(-T_o\rho)\ A \\ (s_qF)^2 &= 4s_q^2\ \exp(-2T_o\rho)\ A^2 \end{aligned}\right\}\ \text{Centrosymmetric, origin at center}$$

$$\left.\begin{aligned} s_qF &= s_q\exp\ (-T_o\rho)\ (A^2 + B^2)^{1/2} \\ (s_qF)^2 &= s_q^2\ \exp(2T_o\rho)\ (A^2 + B^2) \end{aligned}\right\}\ \text{Acentric}$$

Here s_q is the scale factor, T_o is the overall temperature factor coefficient, and ρ is $(\sin\theta/\lambda)^2$.

A and B are computed in space groups P1 or $P\bar{1}$ as follows:

$$A = A_o + \sum_i f_i \exp(-T_i\rho) \sum_j \exp_{ij}\cos_{ij}$$

$$B = B_o + \sum_i fi \exp(-T_i\rho) \sum_j \exp_{ij}\sin_{ij}$$

Here A_o and B_o are fixed atom contributions which may have been computed previously or which may be zero. The subscript i refers to the different atoms in the asymmetric unit while the subscript j refers to the symmetrically equivalent positions to which each ith atom may be transformed. (In the centrosymmetric case j numbers only half the equivalent positions). T_i and f_i are the symmetric temperature factor coefficient and the form factor for each atom. The terms $\cos_{ij}$ and $\sin_{ij}$ are the trigonometric contributions of the ith atom transformed to the jth equivalent position, and $\exp_{ij}$ is the anisotropic temperature factor for this atom. OR XLS2 sets either $\exp(-T_i\rho)$ or $\exp_{ij}$ at unity depending on which kind of temperature factor is to be used.

The trigonometric contribution $\cos_{ij}$ could be computed as

$\cos_{ij} = \cos 2\pi(hx'_{ij} + ky'_{ij} + \ell z'_{ij})$ with a similar expression for $\sin_{ij}$.

Here h, k, and ℓ are the indices and x'_{ij}, y'_{ij}, and z'_{ij} are the coordinates of the ith atom in the asymmetric unit transformed (as indicated by the primes) to the jth equivalent position. OR XLS2 does not do this, however. Instead of transforming the coordinates, the indices h, k, and ℓ are transformed in a way which makes the result identical with the above:

$\cos_{ij} = \cos 2\pi(h'_j x_i + k'_j y_i + \ell'_j z_i + t_j)$ with a similar expression for $\sin_{ij}$.

Here x_i, y_i, and z_i are the (untransformed) coordinates for the ith atom in the asymmetric unit, h'_j, k'_j, and ℓ'_j are the transformed indices, and t_j is a translational term. As an example we will illustrate the transformations used for the general positions of space group $C3_22$.

j	x'_j	y'_j	z'_j	h'_j	k'_j	ℓ'_j	t_j
1	x	y	z	h	k	ℓ	0
2	x-y	-y	-z	h	-h-k	$-\ell$	0
3	y-x	-x	1/3 + z	-h-k	h	ℓ	$\ell/3$
4	-x	y-x	1/3 - z	-h-k	k	$-\ell$	$\ell/3$
5	-y	x-y	2/3 + z	k	-h-k	ℓ	$2\ell/3$
6	y	x	2/3 -z	k	h	$-\ell$	$2\ell/3$

Substitution of these quantities in the two expressions for $\cos_{ij}$ will give identical results.

OR XLS2 permits this symmetry to be introduced in one of two ways: (1) A generalized symmetry routine is used which takes its instructions from symmetry cards which are supplied as data. There is one such card for each j value, and it consists of a statement of the coordinate transformations (as in the left half of the above table). The program then automatically performs the transformations on the indices which are equivalent to the coordinate transformations specified. (2) The user may elect to write his own symmetry routines to transform the indices. Specifications for such routines will be given below. It may be expected that some speed will be gained in this way.

The anisotropic temperature factor, $\exp_{ij}$, is handled similarly. The fundamental expression is

$$\exp_{ij} = \exp\left\{-\left[h^2\beta'_{11_{ij}} + k^2\beta'_{22_{ij}} + \ell^2\beta'_{33_{ij}} + 2hk\beta'_{12_{ij}} + 2h\ell\beta'_{13_{ij}} + 2k\ell\beta'_{23_{ij}}\right]\right\}$$

where $\beta'_{11_{ij}}$, etc. are the six temperature factor coefficients for the ith atom of the asymmetric unit transformed to the jth equivalent position. Again the program makes the computation by transforming the index products rather than the coefficients themselves so that

$$\exp_{ij} = \exp\left\{-\left[(h^2)'_j\beta_{11_i} + (k^2)'_j\beta_{22_i} + (\ell^2)'_j\beta_{33_i} + (2hk)'_j\beta_{12_i} + (2h\ell)'_j\beta_{13_i} + (2k\ell)'_j\beta_{23_i}\right]\right\}.$$

Here $(h^2)'_j$, etc. are the transformed index products which make the two expressions identical.

Rules for obtaining the transformed coefficients $\beta'_{11_{ij}}$, etc. for any space group have been given by H. A. Levy (Acta Cryst. (1956) 9, 679). From these rules it may be deduced that for atoms in general positions $(h^2)'_j = (h'_j)^2$, etc. so that the transformed index products are simply the products of the transformed indices. This is not necessarily true for atoms in special positions, however. The generalized symmetry routine of OR XLS2 computes the products of transformed indices and assumes that $(h^2)'_j = (h'_j)^2$, etc., and therefore <u>the computed anisotropic temperature factor may not be valid for atoms in special positions</u>.

<u>Cells with translational symmetry (centering)</u>

The specification of symmetry in the case of face, end, or body centered cells can be simplified (and the computing time reduced) provided that the reflections which are extinguished by centering are not computed. Similar considerations apply to a rhombohedral cell described by hexagonal coordinates.

In these cases, symmetry cards or routines need be supplied only for positions not related by translation. The scattering factors should then be multiplied by the appropriate integer in the way described below (page 14).

Special positions

We must now consider the ways of handling the computation when atoms are in special positions. The important effects of an atom being in special positions are (a) that the number of these atoms is smaller than if they were in general positions, (b) that there are certain restrictions on the position parameters, and (c) that there may be some restrictions on the anisotropic temperature factor coefficients. No restrictions on symmetric temperature factors are introduced, however.

The ways of handling special positions with OR XLS2 depend on several factors: (1) whether all the atoms are in the same kind of special position, (2) whether the position parameters have a fixed value or whether there is a relationship between two or more coordinates, (3) whether anisotropic temperature factors are used or not, and (4) if used, whether there are (a) no restrictions on the coefficients, (b) certain coefficients fixed at zero, or (c) a relationship between two or more coefficients. H. A. Levy (loc. cit.) has given a rule for determining the restrictions on the anisotropic temperature factor coefficients of atoms in special positions.

Fixed parameters. When coordinates or temperature factor coefficients have fixed values then these values may be put into the list of trial parameters. The parameter selection words are then written so that these parameters are not varied. The symmetry cards are written for the general positions so that anisotropic temperature factors are correctly computed.

Symmetry cards for special positions. If all atoms are in the same kind of special position, and if anisotropic temperature factors are not used, then the correct result will be obtained by using symmetry cards for the special positions. For example, the space group $C3_22$ mentioned above has special positions for $y = x$, $z = 1/3$ with the transformations:

j	x_j'	y_j'	z_j'
1	x	x	1/3
2	0	-x	2/3
3	-x	0	0

This information can be punched on three symmetry cards instead of using the six general positions as data. All coordinates y and z in the parameter input are then irrelevant, and no attempt must be made to vary them.

Writing special patches. It is possible to handle any symmetry situation which can arise by using symmetry cards for the general positions, allowing the generalized symmetry routine to compute the transformed indices and the index products which would be valid for these general positions, and then transferring to a specially written section of code which modifies these transformed indices appropriately. Consider, for example, the special positions mentioned above. The generalized symmetry routine alone would produce the trigonometric argument.

$$h_j' x_i + k_j' y_i + \ell_j' z_i + t_j.$$

Now let us make x_i the independent variable and require that $y_i = x_i$, $z_i = 1/3$. Substituting in the argument we have

$$h_j' x_i + k_j' x_i + \ell_j'/3 + t_j.$$

Now the program will produce this result if we replace h_j' by $h_j'' = h_j' + k_j'$, k_j' by $k_j'' = 0$, ℓ_j' by $\ell_j'' = 0$, and t_j by $t_j' = t_j + \ell_j'/3$. Instructions for programming such a patch will be given below. The parameters y and z will again be irrelevant and must not be varied.

The restrictions on the anisotropic temperature factor coefficients may be handled in a similar way. For the atoms in the above example, Levy's rule shows that $\beta_{22} = \beta_{11}$, $\beta_{23} = -\beta_{13}$. Taking β_{11} and β_{13} as independent the required transformations are:

$$(h^2)_j'' = (h_j^2)' + (k_j^2)'$$

$$(k^2)_j'' = 0$$

$$(\ell^2)_j'' = (\ell^2)_j'$$

$$(2hk)_j'' = (2hk)_j'$$

$$(2h\ell)_j'' = (2h\ell)_j' - (2k\ell)_j'$$

$$(2k\ell)_j = 0$$

Again β_{22} and β_{23} are irrelevant and must not be varied. It is desirable, however, after the parameters have been adjusted to reset $\beta_{22} = \beta_{11}$ and $\beta_{23} = -\beta_{13}$. This is necessary if the test for positive definite temperature factor coefficients is to be valid. Specifications for the code patch to do this resetting are given below.

Note that there is no reason why a combination of the fixed parameter and special patch methods may not be used. In the above example the z parameters could be fixed at 1/3 while the patch handles the y = x restriction. Note also that it may be possible to choose a coordinate system which simplifies the restrictions on the parameters.

Correcting the number of atoms. The program as written always sums over all the equivalent positions as specified by the symmetry cards. Thus the effective number of times an atom is included is equal to the number of symmetry cards (or the number of user's symmetry routines) for acentric structures and twice that number for centrosymmetric structures. If the symmetry cards (or routines) describe the general positions then atoms in special positions may be put in correctly by scaling their scattering factors by the appropriate integer. In the X-ray case this may be done when the form factor tables are prepared, and in the neutron case the scattering factor in the parameter table is adjusted. When the symmetry cards are written for the special positions directly then no modification of the scattering factor is necessary.

Specifications for user's symmetry routines

1. Entry at XD1. OR XLS2 automatically transfers to XD1 if sense card specifies "symmetry routine supplied by user".
2. Write μ routines where μ is the number of equivalent positions for acentric computation or one half this number for centrosymmetric computation.
3. The program transfers to XD1 μ times for each reflection and the user must arrange to enter each of his routines once per reflection. For this purpose Index 4 contains μ, μ-1, μ-2 ..... 1 on the first and subsequent entries.
4. The indices (floating point) of the reflection are found at M1, M2, and M3 (see program listing for addresses).
5. The jth routine must store t_j, h'_j, k'_j, and ℓ'_j (floating point) at T12-T15.
6. If anisotropic temperature factors are to be used the routine must also store $(h^2)'_j$, $(k^2)'_j$ .... $(2k\ell)'_j$ (floating point) at T16-T21.
7. OR XLS2 does not destroy the transformed indices so that subsequent entries may make use of the values previously obtained.
8. Index 2 is available. If indices 1 or 4 are used they must be saved and restored.
9. Return to XE.
10. Set the address in T5 to that of the last location used by the symmetry routines or other additions to the code.
11. Assemble routines and insert in the binary deck between OR XLSD and OR XLSE.
12. On the Sense Card specify that user's symmetry routines are to be used.

The following example illustrates the symmetry routines for space group $C3_22$ using symmetric temperature factors. The required transformations have been tabulated above.

```
        REM     EXAMPLE ØF USERS SYMMETRY RØUTINES
        ØRG     (Fill in address)
T5      PZE     THIRD                       LAST ADDRESS USED
XD1     TRA     A, 4                        ENTRY
        TRA     A
        TRA     B
        TRA     C
        TRA     D
        TRA     E
        TRA     F
A       STZ     TJ
        LXA     I3, 2
A1      CLA     H + 3, 2
        STØ     HJ + 3, 2
        TIX     A1, 2, 1
        TRA     XE
B       CLS     H
        FSB     K
        STØ     KJ
        CLS     L
        STØ     LJ
        TRA     XE
C       CLA     KJ
        STØ     HJ
        CLA     H
        STØ     KJ
        LDQ     L
        STQ     LJ
        FMP     THIRD
        STØ     TJ
        TRA     XE
D       CLA     K
        STØ     KJ
        CLS     L
        STØ     LJ
        TRA     XE
E       CLA     HJ
        STØ     KJ
        CLA     K
        STØ     HJ
        CLA     L
        STØ     LJ
        CLA     TJ
        FAD     TJ
        STØ     TJ
        TRA     XE
F       CLA     K
        STØ     HJ
        CLA     H
        STØ     KJ
        CLS     L
        STØ     LJ
        TRA     XE
```

```
THIRD     DEC     0.333333
H         EQU                          M1
K         EQU                          M2
L         EQU                          M3
TJ        EQU                          T12
HJ        EQU     (Fill in             T13
KJ        EQU      addresses)          T14
LJ        EQU                          T15
I3        EQU
XE        EQU
          END     0
```

Specifications for patch to handle special positions.

1. Insert a transfer at XI.
2. Patch is probably located somewhere after T5 at end of program. XD1 has no significance if general symmetry routine is used.
3. The program reaches XI ν times for each of the μ values of j. Here ν is the number of atoms in the asymmetric unit and μ is the number of symmetry cards. At each of the ν entries for a given j index 4 contains $i = \nu, \nu - 1, \nu - 2, \ldots 2, 1$.
4. Before reaching XI with a new j value the transformed indices t_j, h_j', k_j', and ℓ_j' have been stored in locations T12-T15 by the generalized symmetry routine in accordance with the symmetry cards. If anisotropic temperature factors are specified then the products of these transformed indices, $(h_j')^2$, $(k_j')^2$, ... $2(h_j')(\ell_j')$, and $2(k_j')(\ell_j')$, have been stored in locations T16-T21.
5. The patch must modify these transformed indices according to the restrictions placed on the parameters by having atoms in special positions. Note that on subsequent entries for a given j value the transformed indices have not been changed but are as they were at the previous exit from the patch. Only when the value of j changes is the generalized symmetry routine re-entered. At this time the transformed indices and products are reset according to the next symmetry card.
6. If any index registers are used they must be saved and restored.
7. Return to XI + 1.
8. Set the address in T5 to that of the last location used by the patch or any other additions.
9. Assemble the patch and insert in the binary deck between OR XLSD and OR XLSE.
10. On the sense card specify that the generalized symmetry routine is to be used (unless user's routines have also been written).

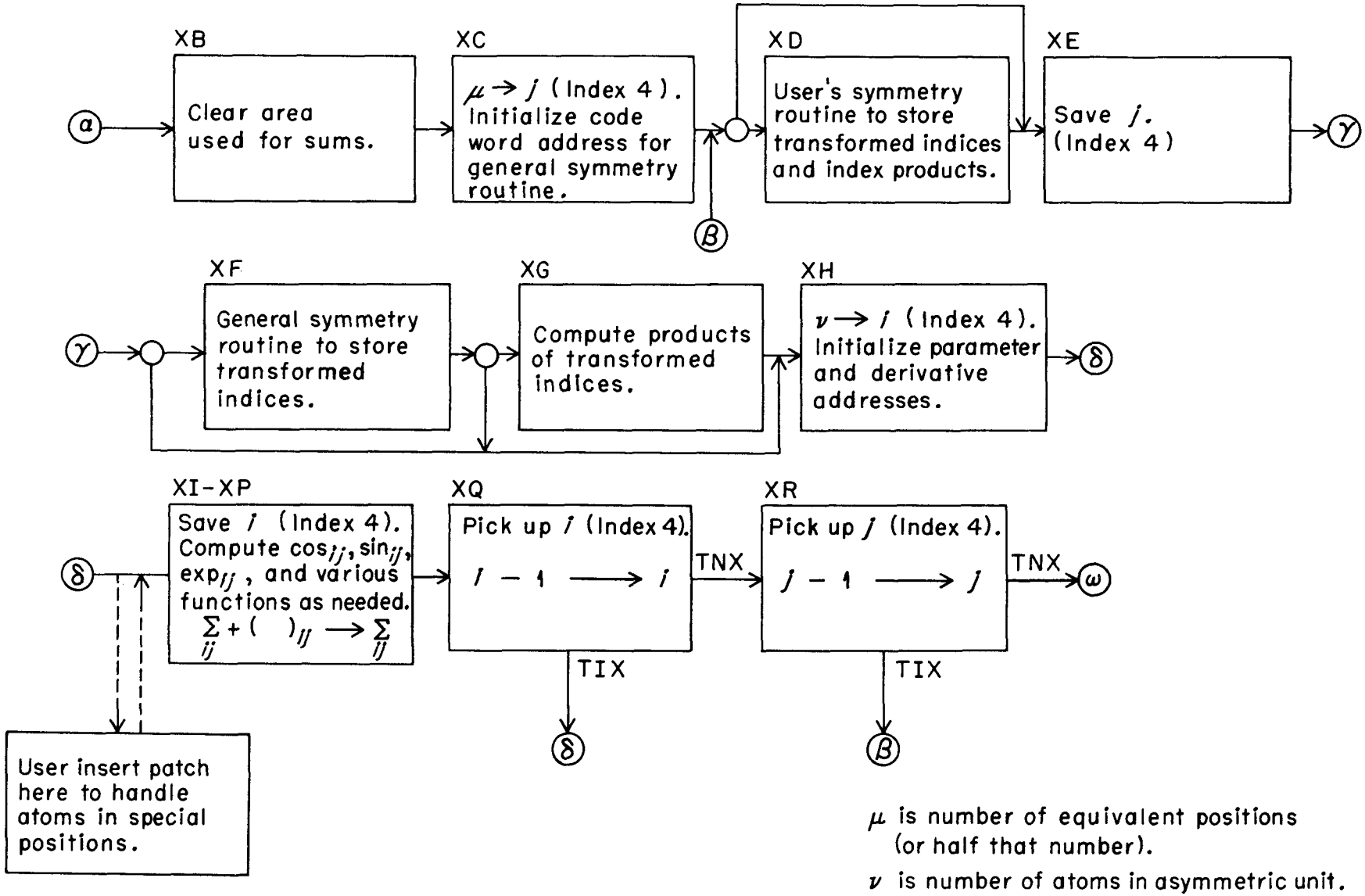
The following example illustrates the use of the patch for a hypothetical structure with one kind of atom in the general positions of $C3_22$ and two more kinds of atoms in the special positions with y = x and z = 1/3 mentioned above. The atoms in general positions will be listed first in the parameter table with the other two following. We select x as the independent variable for the atoms in special positions and fix their z parameters at 1/3. For these atoms the effect on the transformed indices has been discussed above.

```
            REM     SYMMETRY PATCH FØR SPECIAL PØSITIØNS
            ØRG     (Fill in address)
XI          TXL     A, 4, 2                 DØ NØT TRANSFER ØN FIRST ATØM
            ØRG     (Fill in address)
T5          PZE     B                       LAST ADDRESS USED
A           TXL     XI + 1, 4, 1            RETURN FØR THIRD ATØM
            CLA     HJ
            FAD     KJ
            STØ     HJ
            STZ     KJ
            CLA     HHJ
            FAD     KKJ
            STØ     HHJ
            STZ     KKJ
            CLA     2HLJ
            FSB     2KLJ
            STØ     2HLJ
            STZ     2KLJ
B           TRA     XI + 1
HJ          EQU                             T13
KJ          EQU                             T14
HHJ         EQU     (Fill in                T16
KKJ         EQU      addresses)             T17
2HLJ        EQU                             T20
2KLJ        EQU                             T21
            END     0
```

Specifications for patch to reset relationships between parameters.

1. At XWP insert transfer to reset position coordinates. Such resetting serves no essential purpose in the program as now written.
2. At XWQ insert transfer to reset anisotropic temperature factor coefficients. If symmetric temperature factors are used this transfer will automatically be bypassed.
3. Start these patches at end of program after T5 in locations which do not interfere with other patches.
4. On first entry to either patch index 1 contains ν, the number of atoms in the asymmetric unit. On subsequent entries it contains $\nu - 1$, $\nu - 2$, ... 2,1. Index 2 contains the complemented address of the form factor or form factor indicator for each atom so that the parameters of the atom under consideration are found as follows:

Parameter	Address and tag
x_i	1,2
y_i	2,2
z_i	3,2
β_{11i}	4,2
⋮	⋮
β_{13i}	8,2
β_{23i}	9,2



μ is number of equivalent positions (or half that number).

ν is number of atoms in asymmetric unit.

SECTION OF OR XLS2 RELEVANT TO SYMMETRY CONSIDERATIONS

5. Write the patch to reset the relationships between the parameters of atoms in special positions. Parameters are in floating point. Index 4 is free.
6. Return to XWP + 1 and XWQ + 1 after each patch.
7. Set the address in T5 to that of last location used by any patch or symmetry routine.
8. Assemble patches and insert in the binary deck between OR XLSD and OR XLSE.

The following is an example of the patches which would be used with the structure of the previous example. Note that this resetting is done <u>after</u> the parameters are printed but <u>before</u> the test for positive definite temperature factors is made.

```
        REM     PATCH TØ RESET PARAMETERS
        ØRG     (Fill in address)
XWP     TXL     C, 1, 2
        ØRG     (Fill in address)
XWQ     TXL     D, 1, 2
        ØRG     (Fill in address)
T5      PZE     E
        ØRG     (Fill in address)
C       CLA     1, 2
        STØ     2, 2
        TRA     XWP + 1
D       CLA     4, 2
        STØ     5, 2
        CLS     8, 2
        STØ     9, 2
E       TRA     XWQ + 1
        END     0
```

PROCEDURE WHEN SINGULAR MATRIX IS FOUND

The programmed stop in XMC of OR XLS4 indicates that the matrix of the normal equations is singular. This means that the program is attempting to adjust more parameters than are uniquely determined by the observations. Some of the ways in which this can occur will be listed:

1. Error in preparing parameter selection cards.
2. Attempting to vary more parameters than there are observations. An error in the weighting scheme or rejection test could cause this difficulty.
3. Attempting to vary some undetermined parameter (e.g., a z coordinate when hk0 data alone is used).
4. Attempting to vary a parameter which should be fixed because an atom is in a special position.
5. Attempting to vary redundant parameters (e.g., varying the overall temperature factor when all individual atom temperature factors are also varied, or varying the coordinates of all atoms when the origin is not fixed by the symmetry).

6. Attempting to vary parameters which are redundant because of overlapping atoms when data is for a projection. (Unless the overlap is exact this would be expected to produce very large parameter changes rather than a singularity stop.)

Operating procedure when matrix is singular.

1. Take octal dump of last 300 words of core storage.
2. Get off machine.
3. Hold tapes 4 and 5.
4. List tape 3.
5. After locating trouble get back on the machine using operating procedures B, C, D, or E.

Locating the trouble

The matrix as taken from a core dump at this point has been partially inverted. The original matrix may be taken from tape 5 if desired by means of OR XLSN (see page 38). However the vector of the normal equations is available in the dump at the location specified in K12. A zero element in this vector very probably means that the corresponding derivative was zero for all the observations. This could occur for reasons 1, 3, or 4 listed above. If all elements are zero this could mean an error in the weighting scheme or rejection test.

The parameter selection words can also be found in the dump at a location specified in K15. There are two parameter selection words for each parameter selection card, and each binary digit of the former corresponds to one card column.

DATA PROCESSING AND WEIGHT CALCULATION WITH OR XLS1

If the user wishes to compute estimated standard errors according to some formula or to perform on each reflection other preliminary data reduction operations such as scaling, taking a square root, etc., he may do so by writing a section of code according to the following specifications. Note that some of the symbols used in XLS1 are reused with different meansing in XLS2. The programmer should be careful to refer to addresses obtained from the listing of XLS1.

1. Start code at XH.
2. Available space includes 64 locations at XI with additional space at the end of the memory if required.
3. The following data is available in binary floating point:
   a. Cell data at D2-D7.

b. Data from observation card at M1-M5 (unchanged).

c. $(\sin \theta/\lambda)^2$ at M7.

d. Any desired floating point data typed in columns 55-63 and 64-71 of each observation card are found at T13 and T14, respectively.

4. To function as a weight calculator the code must store the standard error (not the weight) of F or F^2 at M5. The program later computes $\sqrt{w} = 1/\sigma$ for $\sigma \neq 0$ ($w = 0$ if $\sigma = 0$).

5. Exit to XJ.

6. Code should be assembled on absolute binary cards and inserted between OR XLSA and OR XLSB.

REJECTING OBSERVATIONS BY MEANS OF A REJECTION TEST

If it is desired to omit from the least squares treatment observations which fail to satisfy some criterion (e.g., reflections with F(calc) much smaller than F(obs)) the user may write a rejection test according to the specifications given below. Reflections rejected by this test will be marked with a single asterisk (*) in the structure factor output. The only effect of this test is to cause the reflection to be ignored when the normal equations are set up. If the reflection passes the test in subsequent cycles it will be reincluded.

Specifications for rejection test

1. Start rejection test at XAX. There are 66 locations available. If more space is needed use the area following T5 and change the address in T5 accordingly.

2. Data available for each observation includes the information in locations M1-M13, part of which is the input data and part of which has just been computed. In the listing of these locations "OBS" and "CALC" refer to F(obs) and sF(calc) or F^2(obs) and s^2F^2(calc), whichever is being used. M14 contains the rejection indicator from the previous cycle, if any.

3. All index registers are available to the programmer.

4. If the reflection is to be accepted (i.e., included in setting up the normal equations) store a zero at M14. If the reflection is to be rejected store something other than zero at M14.

5. Return to XAXX.

6. The test should be assembled on absolute binary cards and inserted between OR XLSD and OR XLSE.

UTILITY ROUTINES

OR XLS1-5 includes several routines which may be of interest to the user. A few of them will be described here.

RCD. Card programmer transfer. This routine reads the 9L word from a card and transfers to that word. This 9L word may be a transfer order, and such transfer cards are used to direct the course of the program. The location to which 9L is copied is RCD-1 so that a sequence of non-transfer instructions may be performed from a sequence of cards. Most of the programmed stops in OR XLS1-5 are coded to HTR RCD.

LDCD. Load self-loading cards. This routine clears the index registers and simulates the function of the load card button on the console.

DUMP is an octal and floating decimal off-line dump of the temporaries of OR XLS1-2. It is not available for use with OR XLS3-5. Transfer cards labeled OR XLSM are available, and these may be inserted in the deck at points where they will be read by the RCD routine, i.e., immediately preceeding another such transfer card. After the dump is completed control is returned to the RCD routine, and the next transfer card is read so that the program proceeds without stops. Some of the positions where OR XLSM may be inserted in the card decks are given in the section on operating procedure (pages 33-38). Attempting to dump when OR XLS3-5 are in the memory cause the program to return to RCD and read the next card without dumping.

The initial and final addresses to be dumped are fixed by the program, but they can be changed by means of binary correction cards.

DATA DECKS

Data deck 1. Input for the preliminary processing segment, OR XLS1.

1. Title
2. Reciprocal cell data.
3. Form factor tables unless problem is a neutron diffraction one.
4. Reflection data unless this is on BCD tape. In either case this data is terminated either by a blank field (but with "R" in column 72) or an end of file (i.e., an empty hopper in card reader).

Data deck 2. Input for OR XLS2 when data is not in memory.

1. Title
2. Sense card
3. Symmetry cards if general symmetry routine is used
4. Reciprocal cell data
5. Trial parameters
6. Key card and parameter selection cards if least squares refinement is being made.

Data deck 3. Input for OR XLS2 when some of the data is already in the memory from previous cycles.

1. Title
2. Sense card. Any individual sense card field which is left blank will cause that sense indicator to keep its value from the previous cycle.

*3. Symmetry cards if general symmetry routine is used

*4. Reciprocal cell data

*5. Trial parameters

*6. Key card and parameter selection cards if least squares refinement is being made.

*Note: If the data from the previous cycle is to remain unchanged each of these groups of data cards may be replaced by one card which is blank except for the correct identification in column 72. CAUTION: Changing the number of scale factors changes the memory location of the parameters and of the symmetry data so that these cards must be supplied in this case.

DETAILS OF DATA INPUT

All input data except the parameter selection cards are converted by means of GL FILE to fixed point integers or floating point numbers with the form of conversion defined by the program. The field in which each entry is to be punched is specified below. The format in which a number should be punched is indicated by the following paragraphs from the GL FILE write-up:

Fixed point integers

The routine examines the characters in the field, working from left to right, and discards all characters until a digit or a minus sign is encountered. This defines the beginning of the number and the next non-digit character (or the end of the field) defines the end of the number. Thus minus signs should immediately precede the number; plus signs may be omitted.

Floating point numbers

Working from left to right the first minus sign, decimal point, or digit encountered defines the beginning of the mantissa; the next non-digit (other than a point) defines the end of the mantissa. The routines then proceed to examine the rest of the field for an exponent in the manner described under the integer operation. If no exponent appears in the field, the routine assumes an exponent of zero. Thus minus signs should immediately precede both mantissa and exponent; plus signs may be omitted.

Examples

1						7
2						
				-	4	
	1	2	5			
-	5					

Fixed Point Integers

1								9
		4						
					2	.	6	6
	-	7	7	E	-	2		
8	.	5	0	1	(	5	)	

Floating Point Numbers

Card identification

Each data card except for the parameter selection cards has an identifying letter punched in column 72. As each data card is read this letter is checked before any of the data is converted. An incorrect letter causes a stop which is monitored on the printer. If the error is located it is only necessary to put the deck back in the reader starting with the corrected data card. Pushing START causes the program to transfer back to the read order on which it stopped.

If it is the identification letter and not the card which is in error the test can be bypassed by turning on sense switch 6. It will then be necessary to put back in the reader the card on which the stop occurred and to START. Subsequent tests will be bypassed as long as sense switch 6 is left on.

Title card

The first card in each data deck.

Columns

1-71	The Hollerith information from these 71 columns is used unchanged as a heading for the output.
72	The identifying letter T.

Example:

1	71	72
2/20/59 HYDROGEN PEROXIDE, CYCLE 1		T

Reciprocal cell data card

One card included in each of data decks 1 and 2.

Columns

1-9	Integer n_f, the number of different X-ray form factor tables to be used. For neutron diffraction make $n_f = 0$. This field is relevant only in data deck 1. It must be the same as columns 19-21 of the sense card (see below).
10-18	Floating point a^*, the reciprocal lattice constant defined so that $\underset{\sim}{a} \cdot \underset{\sim}{a}^* = 1$ (not $\underset{\sim}{a} \cdot \underset{\sim}{a}^* = \lambda$).
19-27	Floating point b^*.
28-36	Floating point c^*.
37-45	Floating point $\cos \alpha^*$.
46-54	Floating point $\cos \beta^*$.
55-63	Floating point $\cos \gamma^*$.
72	The identifying letter C.

Example:

1 9	10 18	19 27	28 36	37 45	46 54	55 63	72
3	.2451	.5103	.4422	0	.1751	0	C

Form factor tables for X-ray problems

Each table consists of four cards and the program reads n_f such tables where n_f is given in columns 1-9 of the reciprocal cell data card. No form factor tables are used for neutron problems. The 32 form factors for $\sin \theta/\lambda$ from 0.00 to 1.55 in intervals of 0.05 are listed in reverse order. Values of the form factor for $\sin \theta/\lambda$ out of range of the problem may be inserted as zeros.

Card	Columns	
1	1-9	Floating point form factor for $\sin \theta/\lambda = 1.55$
	10-18	Floating point form factor for $\sin \theta/\lambda = 1.50$
	19-27	Floating point form factor for $\sin \theta/\lambda = 1.45$
	28-36	Floating point form factor for $\sin \theta/\lambda = 1.40$
	37-45	Floating point form factor for $\sin \theta/\lambda = 1.35$
	46-54	Floating point form factor for $\sin \theta/\lambda = 1.30$
	55-63	Floating point form factor for $\sin \theta/\lambda = 1.25$
	64-71	Floating point form factor for $\sin \theta/\lambda = 1.20$. (Note that this field is one column narrower than the others.)

Card	Columns	
.	72	The identifying letter F.
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.
4	55-63	Floating point form factor for sin θ/λ = 0.05
	64-71	Floating point form factor for sin θ/λ = 0.00
	72	The identifying letter F.

Example:

1 9	10 18	19 27	28 36	37 45	46 54	55 63	64 71	72
0	0	0	0	0	1.144	1.182	1.220	F
1.258	1.296	1.335	1.374	1.418	1.462	1.514	1.566	F
1.634	1.714	1.813	1.944	2.112	2.338	2.631	3.010	F
3.492	4.094	4.814	5.634	6.482	7.250	7.796	8.000	F

Reflection data cards

One card for each reflection observed or for each structure factor to be computed. These reflections may be put in in any desired sequence. The cards may be included in data deck 1, or they may be copied onto BCD tape before loading. In either case this set of data is terminated either by a card blank except for an R in column 72 or by an end of file (i.e., an empty hopper in the card reader).

Columns	
1-9	Floating point index h.
10-18	Floating point index k.
19-27	Floating point index ℓ.
28-36	Floating point observed values of $\|F\|$ or F^2, whichever is being refined. For structure factor calculations this field need not be punched. If it is omitted then a 2 should be punched on the sense card (see below) in columns 16-18 to indicate that this field is to be ignored.
37-45	Floating point σ, the standard error of $\|F\|$ or F^2, whichever is being refined. The least squares weight of a reflection will be $w = 1/\sigma^2$ for $\sigma \neq 0$ (or $w = 0$ for $\sigma = 0$). If an error computing program has been added by the user then an error need not be punched. Nor need an error be punched for structure factor calculations.

Column

46-54 Integer q where q = 1, 2, 3 ....r and s_q is the scale factor to be used in computing this reflection. If this field is left blank the program will make q the same as for the previous reflection. This field must not be blank on the first reflection card read.

55-63 Floating point extra input 1. Any data punched in this field will be stored at T13 for use by an error calculating or data processing routine written by the user.

64-71 Floating point extra input 2. Any data punched in this field will be stored at T14 for the purpose described above.

72 The identifying letter R.

Example:

1 9	10 18	19 27	28 36	37 45	46 54	55 63	64 71	72
2	3	-5	17.2	2.5	2			R
10	0	0	4.5	1.0				R
5	4	1	3.1	1.0				R
-3	1	1	0	1.0	1			R
2	5	0	7.2	1.5				R
								R

Sense card

One such control card is read at the beginning of each cycle of least squares. Directly after reading this card the program prints on-line a summary of the control instructions which serves as an immediate check and which may be saved for reference.

Columns

1-3 Integer 1, 2, 3, or 4, the mode number:
(1) Compute fixed atom contributions.
(2) Compute structure factors s_qF or $(s_qF)^2$.
(3) Conventional least squares.
(4) Least squares cycle using derivatives and inverse matrix from previous mode 3 cycle. When this mode is used the kind of temperature factor and the parameter selection cards must be the same as those of the previous mode 3 cycle. Any number of mode 4 cycles may follow one mode 3 cycle.

4-6 Integer 1 or 2:
(1) Compute and base refinement on s_qF.
(2) Compute and base refinement on $(s_qF)^2$.

7-9 Integer 1, 2, or 3, the type of individual atom temperature factor.
(1) Isotropic or symmetric.
(2) Anisotropic.

Columns

(3) Start with symmetric temperature factors and convert to anisotropic form before refining. The symmetric coefficients may be left from the previous cycle or they may be read from the parameter cards. The parameter selection cards should be made up on the basis of six anisotropic coefficients per atom.

10-12 Integer 1, 2, or 3, the extent of BCD structure factor output desired:
(1) List results for all reflections.
(2) List results only for reflections which fail rejection test (supplied by user) or for which (obs-calc)/(error) > 2.
(3) No structure factor output.

13-15 Integer 1 or 2, but this field is irrelevant except in mode 2:
(1) Binary output tape is to be written.
(2) No binary output tape to be written.

16-18 Integer 1 or 2, but this field is irrelevant except in mode 2:
(1) F(obs) or F^2(obs) has been punched on reflection cards and is to be put out with the computed structure factors and used to compute the R factors.
(2) F(obs) or F^2(obs) is to be ignored if punched and no R factors are to be computed.

19-21 Integer n_f, the number of kinds of X-ray form factors. This must be zero for neutron diffraction, and n_f must be the same as that punched in columns 1-9 of the reciprocal cell data card, data deck 1.

22-24 Integer ν, the number of atoms in the asymmetric unit.

25-27 Integer 1 or 2, the kind of symmetry:
(1) Centrosymmetric with origin at symmetry center.
(2) Acentric.

28-30 Integer μ, the number of symmetrically equivalent positions for acentric computations or half that number for centrosymmetric computations. This is the number of symmetry cards or user's symmetry routines.

31-33 Integer 1 or 2, choice of symmetry routines:
(1) Use the general symmetry routine which is built into program and define symmetry with μ symmetry cards. Integer 1 should be specified even if code patches are written to handle special positions.
(2) Only the μ symmetry routines supplied by the user are to be applied. No symmetry cards are to be read.

34-36 Integer r, the number of scale factors. This must be at least one. There is no harm in including more scale factors than are actually used provided that no attempt is made to adjust the irrelevant ones.

72 The identifying letter S.

Example:

1	3 4	6 7	9 10	12 13	15 15	18 19	21 22	24 25	27 28	30 31	33 34	36	72
3	1	2	1			0	5	1	2	1	3		S

Symmetry cards

When the general symmetry routine is to be used μ symmetry cards are included in data deck 2. Each card describes one transformation of the atomic coordinates. For acentric structures μ is the number of equivalent positions. For centrosymmetric structures μ is half this number with pairs of positions related by a center being included only once.

CAUTION: The general symmetry routine can be assumed to give correct results (a) if all atoms are in general positions, or (b) if all atoms are in the same kind of special positions and only symmetric temperature factors are used. In all other cases consult the section on Symmetry Considerations for the correct procedure.

Column

1-15	The expression for the transformed coordinate x' as follows:
1-11	Floating point translational part of x' or blank.
12	Hollerith -, +, or blank. The sign associated with the symbol in column 13. Blank and + are equivalent.
13	Hollerith X, Y, Z, or blank.
14	Hollerith -, +, or blank. The sign associated with the symbol in column 15. Blank and + are equivalent.
15	Hollerith X, Y, Z, or blank. Note that columns 12 and 13 are exactly equivalent to 14 and 15. Thus the transformation x' = 1/2 - x may be punched

1	11	12	13	14	15
.5		-	X		

or

1	11	12	13	14	15
.5				-	X

.

Note that the expression x' = 2x must be treated as x' = x + x.

16-30	The expression for the transformed coordinate y' as follows:
16-26	Floating point translational part of y' or blank.
27-30	Hollerith sign, symbol, sign, symbol as described above.
31-45	The expression for the transformed coordinate z' as follows:
31-41	Floating point translational part of z' or blank.
42-45	Hollerith sign, symbol, sign, symbol as described above.
72	The identifying letter M.

Example: The six symmetry cards for space group $C3_22$ (see page 10) may be punched as follows:

1	11	12	13	14	15	16	26	27	28	29	30	31	41	42	43	44	45	72
			X						Y						Z			M
			X	-	Y			-	Y					-	Z			M
			Y	-	X			-	X			.333333		+	Z			M
		-	X						Y	-	X	.333333		-	Z			M
		-	Y						X	-	Y	.666667		+	Z			M
			Y						X			.666667		-	Z			M

Trial parameter cards

These include r scale factor cards, one overall temperature factor card, and ν atom parameter cards where ν and r are punched on the sense card (see above). These cards will be described separately.

Scale factor cards

Cards are read in the order s_1, s_2, ...s_q ....s_r where q is the scale factor identification punched in columns 46-54 of the reflection data cards. Note that s_q multiplies the calculated F, not the observed F.

Column

1-9 Floating point scale factor, s_q.

72 The identifying letter P.

Overall temperature factor card

Column

1-9 Floating point T_o, the coefficient for the overall temperature factor $\exp(-T_o \sin^2\theta/\lambda^2)$. T_o may be zero or any positive number. Do not leave blank.

72 The identifying letter P.

Atom parameter cards

One card for each atom in the asymmetric unit.

Column

1-7 For X-ray problems ($n_f \neq 0$) this is an integer from one to n_f which identifies the form factor to be used. The form factors are numbered in the order in which the form factor tables were read from data deck 1.

For neutron problems ($n_f = 0$) this is the floating point neutron scattering factor itself.

8-14 Floating point coordinate x_i.

15-21 Floating point coordinate y_i.

22-28 Floating point coordinate z_i.

For symmetric temperature factors (or for symmetric converted to anisotropic before refining):

Columns

29-35 Floating point T_i, the coefficient for the individual atoms isotropic temperature factor $\exp(-T_i \sin^2\theta/\lambda^2)$. T_i may be zero or any positive number.

36-70 Irrelevant.

72 The identifying letter P.

For anisotropic temperature factors:

Columns

29-35 Floating point β_{11i}, a coefficient in the expression for the anisotropic temperature factor

$$\exp\left[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + 2\beta_{12}hk + 2\beta_{13}h\ell + 2\beta_{23}k\ell)\right].$$

36-42 Floating point β_{22}.

43-49 Floating point β_{33}.

50-56 Floating point β_{12}.

57-63 Floating point β_{13}.

64-70 Floating point β_{23}.

72 The identifying letter P.

Example: The parameter cards for an X-ray problem with two scale factors, three atoms in the asymmetric unit, and symmetric temperature factors might be as follows:

1 – 9		72
.954		P
1.015		P
0		P

1 – 7	8 – 14	15 – 21	22 – 28	29 – 35		72
2	.4713	-.2521	.9412	1.75		P
2	.5433	.1112	-.1043	1.25		P
1	.2710	.4544	.3315	.70		P

Key card

One card included in data deck 2 for least squares (modes 3 or 4). This card is not used in the calculation of fixed atom contributions or structure factors (modes 1 or 2).

Columns

1-6 Integer n, the number of parameters to be adjusted. This is equal to the number of ones punched on the parameter selection cards. This number must be greater than zero and must not exceed the limit set by the memory capacity (see page 4).

7-12 Integer, the number of parameter selection cards which follow.

72 The identifying letter K.

Example:

1 6	7 12		72
57	2		K

Parameter selection cards

These cards follow the key card (see above) and the number of parameter selection cards must be the integer punched in columns 7-12 of that card. Their purpose is to specify the parameters which are to be adjusted by least squares.

Consider the entire list of parameters including the r scale factors, the overall temperature factor coefficient, and the individual atom parameters to be arranged in that order. There are either five or ten atom parameters per atom including the form factor, the three coordinates, and the one or six temperature factor coefficients (depending on whether symmetric or anisotropic temperature factors are being used). Each column of a parameter selection card corresponds to one parameter, the first scale factor to column one, the next to column two, etc., for the first 72 parameters. If there are more than 72 parameters the association is continued on the next card, parameter 73 corresponding to column one, etc.

If a parameter is to be varied a one is punched in the corresponding column, otherwise a zero or blank is punched. (Actually, all rows but the 1 row are ignored by the program.)

There is no identifying letter to be punched in column 72.

Note that in both the X-ray and neutron case the scattering factor is considered to be a parameter. The neutron scattering factor may be adjusted by least squares, but varying an X-ray scattering factor must not be attempted.

Examples: Consider an X-ray problem with three scale factors, two atoms in the asymmetric unit, and symmetric temperature factors. Only hk0 zone data are to be used and only the first scale factor will be adjusted. The parameter list and corresponding parameter selection card is:

s_1	s_2	s_3	T_0	f_1	x_1	y_1	z_1	B_1	f_2	x_2	y_2	z_2	B_2
1					6	7					12	13	
1	0	0	0	0	1	1	0	1	0	1	1	0	1

If the same problem were set up for anisotropic temperature factors the parameter list and the corresponding parameter selection card might be:

s_1	s_2	s_3	T_0	f_1	x_1	y_1	z_1	β_{ij1} 11	22	33	12	13	23	f_2	x_2	y_2	z_2	β_{ij2} 11	22	33	12	13	23
1					6	7					12	13					18	19					24
1	0	0	0	0	1	1	0	1	1	0	1	0	0	0	1	1	0	1	1	0	1	0	0

OPERATING PROCEDURE

*Inserting OR XLSM immediately preceding a deck marked with an asterisk will cause the program to put out via tape unit 3 an octal and floating decimal dump of the temporaries from the preceeding calculation. This does not interfere with the computation in any way.

A. Data processing following by least squares or by structure factor calculation.

Card deck

1. OR XLSA, B (red)
2. Data deck 1
*3. OR XLSC, D, E (orange)
4. Data deck 2

   For calculating only structure factors (mode 2) the cards after this point are not needed.

*5. OR XLSF (yellow)

   If only one cycle is to be run the cards after this point are not needed.

6. OR XLSG (brown)
7. Data deck 3
*8. OR XLSH (blue)
9. For each additional cycle repeat decks 6, 7, and 8.

Operating Instructions for Case A

1. If tape input of reflection data is to be used mount it on unit 4.
2. Blank tapes on units 3 and 5.
3. Sense switch 1: Off for tape input,
   On for card input.
4. Sense switch 2: Off if BCD output from XLS1 is desired,
   On to suppress this output.

5. Sense switch 3: Off for on-line output of F or F^2,
   On to suppress this on-line output.
   (Off-line output is unaffected by this setting.)

6. Sense switch 4: Off for on-line output of parameters,
   On to suppress this on-line output.
   (Off-line output is unaffected by this setting.)

7. Sense switch 6: Off normally,
   On to bypass data identification check.

8. Ready printer with SHARE II board.

9. Clear and load cards. Programmed stop at 157_8. This completes OR XLS1. Observations are now on logical tape 5.

10. Switch the tape unit that was 5 to 4. Put a blank tape on unit 5. Start.

11. Programmed stop at 160_8. This is the end of the cycle. Observations, derivatives, and programs are now on logical tape 5 and this may be used as the sole tape input for further cycles. Information on logical tape 4 is unchanged.

12. To start a new cycle switch tape unit that was 5 to 4. Put a blank tape on unit 5. Start. Stops as in step 11 above.

13. Repeat step 12 for as many cycles as desired.

14. List logical tape 3. Program control. Automatic overflow.

15. Hold logical tape 5 to use as the input for further cycles. If for some reason the problem was stopped in mid-cycle it is desirable to hold also logical tape 4. If structure factors were calculated with no binary output then logical tape 4 should be held if further calculations are to be made.

B. Least squares or structure factor calculation when output of OR XLS1 is used as input.

Card deck

1. OR XLSK (red stripe)

2. OR XLSC, D, E (orange)

3. Data deck 2

   For calculating only structure factors (mode 2) the cards after this point are not needed.

*4. OR XLSF (yellow)

   If only one cycle is to be run the cards after this point are not needed.

5. OR XLSG (brown)

6. Data deck 3

*7. OR XLSH (blue)

8. For each additional cycle repeat decks 5, 6, and 7.

C. Least squares or structure factor calculation when the output of a previous least squares cycle is used as the input.

Card deck

1. OR XLSJ (green)
2. Data deck 3

   For calculating only structure factors (mode 2) the cards after this point are not needed.

*3. OR XLSH (blue)
4. OR XLSG (brown)
5. Data deck 3
*6. OR XLSH (blue)
7. For each additional cycle repeat decks 4, 5, and 6.

D. Least squares or structure factor calculation when the output of a previous structure factor or fixed atom contribution calculation is used as the input.

Card deck

1. OR XLSJ (green)
2. Data deck 3 (except that new parameters will be needed if input is from fixed atom contribution calculation)

   For calculating only structure factors (mode 2) the cards after this point are not needed.

*3. OR XLSF (yellow)

   If only one cycle is to be run the cards after this point are not needed.

4. OR XLSG (brown)
5. Data deck 3
*6. OR XLSH (blue)
7. For each additional cycle repeat decks 4, 5, and 6.

Operating Instructions for Cases B, C, or D.

1. Mount binary input tape on unit 4.
2. Blank tapes on units 3 and 5.
3. Sense switch 3: Off for on-line output of F or F^2,
   On to suppress this on-line output.
   (Off-line output is unaffected by this setting.)
4. Sense switch 4: Off for on-line output of parameters,
   On to suppress this on-line output.
   (Off-line output is unaffected by this setting.)
5. Sense switch 6: Off normally,
   On to bypass data identification check.
6. Ready printer with SHARE II board.

7. Clear and load cards.
8. Programmed stop at 160_8. This is the end of the cycle. Observations, derivatives, and programs are now on logical tape 5 and this may be used as the sole tape input for further cycles. Information on logical tape 4 is unchanged.
9. To start a new cycle switch tape unit that was 5 to 4. Put a blank tape on unit 5. Start. Stops as in step 8 above.
10. Repeat step 9 for as many cycles as desired.
11. List logical tape 3. Program control. Automatic overflow.
12. Hold logical tape 5 to use as the input for further cycles. If for some reason the problem was stopped in mid-cycle it is desirable to hold also logical tape 4. If structure factors were calculated with no binary output then logical tape 4 should be held if further calculations are to be made.

E. To get back onto the machine when least squares has given wrong results because wrong parameters were varied.

Card deck

1. OR XLSL (green stripe)
2. Key card and parameter selection cards

*3. OR XLSF (yellow)

If only one cycle is to be run the cards after this point are not needed.

4. OR XLSG (brown)
5. Data deck 3

*6. OR XLSH (blue)

7. For each additional cycle repeat decks 4, 5, and 6.

Operating Instructions for Case E.

1. Mount output from faulty cycle on tape unit 5.
2. Blanks on units 3 and 4. Tape 4 is not written on, but it will receive a rewind order.
3. Follow steps 3 to 12 of the Instructions for Cases B, C, and D.

F. Data processing followed by calculation of fixed atom contribution and then by least squares.

Card deck

1. OR XLSA, B (red)
2. Data deck 1 including form factor tables for fixed and non-fixed atoms.

*3. OR XLSC, D, E (orange)

4. Data deck 2 with parameters of only the fixed atoms and with no key card or parameter selection card.

*5. OR XLSG (brown)

6. Data deck 2 with parameters of only the non-fixed atoms.

*7. OR XLSF (yellow)

If only one cycle is to be run the cards after this point are not needed.

8. OR XLSG (brown)

9. Data deck 3

*10. OR XLSH (blue)

11. For each additional cycle repeat decks 8, 9, and 10.

Operating Instructions for Case F.

1. If tape input of reflection data is to be used mount it on unit 4.

2. Blank tapes on units 3 and 5.

3. Sense switch 1: Off for tape input,
On for card input.

4. Sense switch 2: Off if BCD output from XLS1 is desired,
On to suppress this output.

5. Sense switch 3: Off for on-line output of F or F^2,
On to suppress this on-line output.
(Off-line output is unaffected by this setting.)

6. Sense switch 4: Off for on-line output of parameters,
On to suppress this on-line output.
(Off-line output is unaffected by this setting.)

7. Sense switch 6: Off normally,
On to bypass data identification check.

8. Ready printer with SHARE II board.

9. Clear and load cards. Programmed stop at 157_8. This completes OR XLS1. Observations are now on logical tape 5.

10. Switch the tape unit that was 5 to 4. Put a blank tape on unit 5. Start.

11. Programmed stop at 160_8. Observations and fixed atom contributions are now on logical tape 5. Information on logical tape 4 is unchanged.

12. Switch the tape that was 5 to 4. Put a blank tape on unit 5. Start.

13. Programmed stop at 160_8. This is the end of the cycle. Observations, fixed atom contributions, derivatives, and programs are now on logical tape 5 and this may be used as the sole tape input for further cycles. Information on logical tape 4 is unchanged.

14. To start a new cycle switch tape unit that was 5 to 4. Put a blank tape on unit 5. Start. Stops as in step 13 above.

15. Repeat step 14 for as many cycles as desired.

16. List logical tape 3. Program control. Automatic overflow.

17. Hold logical tape 5 to use as the input for further cycles. If for some reason the problem was stopped in mid-cycle it is desirable to hold also logical tape 4. If structure factors were calculated with no binary output then logical tape 4 should be held if further calculations are to be made.

G. Output of matrix of normal equations or its inverse.

Card deck

1. OR XLSN (orange stripe). (If tape 5 is the output of an incomplete cycle, e.g., after a singular matrix is found, it will be necessary to insert a single absolute binary card immediately preceding the transfer card of OR XLSN. This card should load N, the order of the matrix, in binary into the address part of location 1314_8.

Operating Instructions for Case G.

1. Mount on unit 5 the binary output tape from a least squares cycle, mode 3. (If the tape is from a mode 4 cycle only the inverse matrix can be put out.)
2. Blank tape on unit 3 or this may be the same output tape used for the least squares cycle. It is not rewound before using.
3. Sense switch 5: Off for direct matrix of normal equations,
   On for inverse matrix.
4. Clear and load cards. Stops at 342_8.
5. If more than one matrix is to be put out repeat steps 1 to 4. The program does not reset itself.
6. List tape 3. Program control. Automatic overflow. Hold tape 5 if desired. It has not been written on.

PRELIMINARY TIME ESTIMATES

OR XLS1 with card input of data.

Time = (No. of observations + 50) (7.2×10^{-3} minutes).

OR XLS2 derivative calculation with off-line BCD output.

Time = (No. of observations)(No. of atoms in asymmetric unit)

x (No. of symmetry cards)(1 for centrosymmetric, 2 for acentric)

x (1 for symmetric temp. fact., 2 for anisotropic)(2.9×10^{-4} minutes).

OR XLS3 setting up matrix.

Time = (No. of observations)(No. of parameters varied)^2(4.3×10^{-6} minutes).

OR XLS4 inverting matrix.

Time = (No. of parameters varied)^3(3.6×10^{-6} minutes).

INSTRUCTIONS FOR ASSEMBLING

Binary decks ready for use are available so that it should not often be necessary to assemble the program from the symbolic cards. If such an assembly is made, however, it will be necessary to add to the resulting binary cards certain loaders, relocatable subroutines, tables, and transfer cards which can be obtained from the available binary decks. Reference should be made to the table of binary card decks supplied (pages 39 to 41).

Assembly of OR XLS using SAP3-7 produces only the Utility programs.

Assembly of OR XLS1 produces the program and origin cards for the relocatable subroutines DBD1, FILE, SQRT3, and OUT3 in that order.

Assembly of OR XLS2 produces the program, origin cards for DBD1, FILE, SQRT3, OUT3, and SINEXP, and the loader MU SBL2 with the correct shifting increment.

Assembly of OR XLS3 produces only the program.

Assembly of OR XLS4 produces the program and an origin card for the relocatable subroutine OR SMI.

Assembly of OR XLS5 produces only the program.

Assembly of OR XLS6 produces the program, an origin card for OUT3, and a transfer card.

The various transfer cards will need to be changed only if the memory locations of the first few words in each segment are changed.

BINARY CARD DECKS SUPPLIED

OR XLSA, B (red*)	Type of card	Identification
1. NY RBL1	Self-loading	OR XLSA 00-04
2. UTILITY	Absolute	OR XLSA 05-11
3. OR XLS1	Absolute	OR XLSA 12-36
4. Changes for OR XLS1 (if any)	Absolute	
5. Origin and NY DBD1	Relocatable	OR XLSB 00-08
6. Origin and GL FILE	Relocatable	OR XLSB 09-19
7. Origin and CL SQRT3	Relocatable	OR XLSB 20-22
8. Origin and NY OUT3	Relocatable	OR XLSB 23-41
9. HTR RCD	Transfer	OR XLSB 42
10. TXI START	Transfer	OR XLSB 43

*It is suggested that the user reproduce the cards in the indicated colors.

OR XLSC, D, E (orange)	Type of card	Identification
1. TXI LDCD	Transfer	OR XLSC 00
2. NY RBL1	Self-loading	OR XLSC 01-05
3. OR XLS2	Absolute	OR XLSC 06-99
4. Changes for OR XLS2 (if any)	Absolute	OR XLSD 00-27
5. User's symmetry routines (if any)	Absolute	
6. Origin and NY DBD1	Relocatable	OR XLSE 00-08
7. Origin and GL FILE	Relocatable	OR XLSE 09-19
8. Origin and CL SQRT3	Relocatable	OR XLSE 20-22
9. Origin and NY OUT3	Relocatable	OR XLSE 23-41
10. Origin and SINEXP subroutines	Relocatable	OR XLSE 42-45
11. HTR RCD	Transfer	OR XLSE 46
12. TXI LDCD	Transfer	OR XLSE 47
13. MU SBL2 for TABLES	Self-loading	OR XLSE 48
14. TABLES used by SINEXP	Absolute with nominal origin zero	OR XLSE 49-78
15. TXI START	Transfer	OR XLSE 79
OR XLSF (yellow)		
1. TXI LDCD	Transfer	OR XLSF 00
2. NY RBL1	Self-loading	OR XLSF 01-05
3. OR XLS3	Absolute	OR XLSF 06-13
4. Changes for OR XLS3 (if any)	Absolute	
5. HTR RCD	Transfer	OR XLSF 14
6. TXI START	Transfer	OR XLSF 15
7. TXI LDCD	Transfer	OR XLSF 16
8. NY RBL1	Self-loading	OR XLSF 17-21
9. OR XLS4	Absolute	OR XLSF 22-23
10. Changes for OR XLS4 (if any)	Absolute	
11. Origin and OR SMI	Relocatable	OR XLSF 24-36
12. HTR RCD	Transfer	OR XLSF 37
13. TXI START	Transfer	OR XLSF 38
14. TXI LDCD	Transfer	OR XLSF 39
15. NY RBL1	Self-loading	OR XLSF 40-44
16. OR XLS5	Absolute	OR XLSF 45-48
17. Changes for OR XLS5 (if any)	Absolute	
18. HTR RCD	Transfer	OR XLSF 49
19. TXI START	Transfer	OR XLSF 50
OR XLSG (brown)		
1. TXI START	Transfer	OR XLSG 00
OR XLSH (blue)		
1. TXI KB	Transfer	OR XLSH 00
2. TXI KC	Transfer	OR XLSH 01
3. TXI KD	Transfer	OR XLSH 02

OR XLSJ (green)	Type of card	Identification
1. NY RBL1	Self-loading	OR XLSJ 00-04
2. UTILITY	Absolute	OR XLSJ 05-11
3. HTR RCD	Transfer	OR XLSJ 12
4. TXI KA	Transfer	OR XLSJ 13
OR XLSK (red stripe)		
1. NY RBL1	Self-loading	OR XLSK 00-04
2. UTILITY	Absolute	OR XLSK 05-11
3. HTR RCD	Transfer	OR XLSK 12
OR XLSL (green stripe)		
1. NY RBL1	Self-loading	OR XLSL 00-04
2. UTILITY	Absolute	OR XLSL 05-11
3. HTR RCD	Transfer	OR XLSL 12
4. TXI KF	Transfer	OR XLSL 13
OR XLSM (Manila)		
1. TXI DUMP	Transfer	OR XLSM 00
OR XLSN (orange stripe)		
1. NY RBL1	Self-loading	OR XLSN 00-04
2. OR XLS6	Absolute	OR XLSN 05-15
3. Origin and NY OUT3	Relocatable	OR XLSN 16-34
4. HTR MA	Transfer	OR XLSN 35

ARRANGEMENT OF RECORDS ON BINARY OUTPUT TAPE

From OR XLS1	End of Mode 1 or 2 (if used)	Before loading OR XLS3	Before loading OR XLS4	Before loading OR XLS5	Before correcting parameters	End of cycle
Dummy record	Dump of OR XLS2 program through parameters	Dummy record	→	→	→	Dump of OR XLS2 through corrected parameters
Dummy record	→	→	→	→	→	→
Dummy record	Dump of last 256 words in memory	Dummy record	→	→	→	Dump of last 256 words in memory
Dummy record	→	→	→	→	→	→
Binary data, one record per observation. See next page	→	→	→	→	→	→
End of file	→	→	→	→	→	→
End of file	→	OR XLS2 thru input parameters	→	→	→	→
			OR XLS3 program	→	→	→
			Matrix	→	→	→
				OR XLS4 program	→	→
				Inverse matrix	→	→
					OR XLS5 program	→
					Parameter changes + diagonal elements of inverse	→
					End of file	→

ARRANGEMENT ON TAPE OF BINARY DATA FOR EACH OBSERVATION

	Output of OR XLS1	Output of OR XLS2 Mode 1	Output of OR XLS2 Mode 2	Output of OR XLS2 Mode 3	Output of ORXLS2 Mode 4
M1 h M2 k M3 ℓ M4 Observed F or F^2	Copied	Copied	Copied	Copied	Copied
M5 $1/\sigma = \sqrt{w}$	Computed				
M6 Scale factor identification, q	Copied				
M7 $(\sin\theta/\lambda)^2$ Form factors unless problem is a neutron one	Computed				
M8 Fixed atom A_o M9 Fixed atom B_o	Zero Zero	Computed			
M10 A M11 B M12 Calculated s_qF or $(s_qF)^2$			Computed	Computed	Computed
M13 Observed - calculated M14 Rejection indicator					
M15 $\partial/\partial s$ M16 $\partial/\partial T_o$ Derivatives with respect to atomic parameters (5 or 10 per atom).					Copied

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```
                                                OR-XLS1-5   CRYSTALLOGRAPHIC LEAST SQUARES REFINEMENT
                                                OR-XLS      UTILITY ROUTINES AND INTERSEGMENT PROGRAM
                          00004  U1     EQU 4                   NUMBER OF BINARY INPUT TAPE
                          00005  U3     EQU 5                   NUMBER OF BINARY OUTPUT TAPE
                          00144         ORG 100
      00144  0 02000 0 00165            TRA RCD
      00145  0 02000 0 00171            TRA LDCD
      00146  0 02000 0 00201            TRA WTB
      00147  0 02000 0 00241            TRA RTB
      00150  0 00000 0 00000            PZE
      00151  0 02000 0 00271            TRA KA
      00152  0 02000 0 00304            TRA KB
      00153  0 02000 0 00316            TRA KC
      00154  0 02000 0 00324            TRA KD
      00155  0 02000 0 00332            TRA KE
      00156  0 02000 0 00337            TRA KF
      00157  0 00000 0 00165  KG        HTR RCD                 END OF OR XLS1
      00160  0 00000 0 00165  KH        HTR RCD                 END OF CYCLE. TEMP FACTORS OK.
      00161  0 00000 0 00162  KI        HTR KI1                 END OF CYCLE. TEMP FACTORS NO GOOD.
      00162  0 00000 0 00163  KI1       HTR KI2                    DITTO
      00163  0 00000 0 00165  KI2       HTR RCD                    DITTO
                                            CARD PROGRAMMED TRANSFER
      00164  0 00000 0 00000            PZE
      00165  0 76200 0 00321  RCD       RCD
      00166  0 70000 0 00164            CPY RCD-1
      00167  0 02000 0 00164            TRA RCD-1
      00170  0 00000 0 00165            HTR RCD
                                            LOAD SELF-LOADING CARDS
      00171  0 76200 0 00321  LDCD      RCD
T     00172 -0 73400 0 00000            PDX
      00173 -0 75400 7 00000            PXD 0,7
      00174  0 70000 0 00000            CPY 0
TD    00175  1 00000 0 00177            TXI LDCD+6
      00176  0 00000 0 00171            HTR LDCD                END OF FILE
      00177  0 70000 0 00001            CPY 1
TD    00200  1 00000 0 00000            TXI 0
                                            SUBROUTINE TO STORE BLOCK ON TAPE
      00201  0 50000 4 00001  WTB       CLA 1,4
      00202  0 40000 0 00237            ADD WTB12
      00203  0 62100 0 00215            STA WTB3
      00204  0 62100 0 00222            STA WTB7
      00205  0 50000 4 00001            CLA 1,4
      00206  0 40000 0 00240            ADD WTB13
```

```
00207  0 62100 0 00221          STA WTB6
00210  0 62100 0 00234          STA WTB11
00211 -0 53400 1 00226  WTB1    LXD WTB9,1
00212  0 50000 4 00002  WTB2    CLA 2,4
00213  0 73400 2 00000          PAX 0,2
00214  0 62200 0 00220          STD WTB5
00215  0 76600 0 00220  WTB3    WTB 0                    ADDRESS TO BESET
00216  0 70000 2 00000  WTB4    CPY 0,2
00217  1 77777 2 00220          TXI WTB5,2,-1
00220  3 00000 2 00216  WTB5    TXH WTB4,2,0             DECREMENT TO BE SET
00221  0 76400 0 00200  WTB6    BST 0                    ADDRESS TO BE SET
00222  0 76200 0 00220  WTB7    RTB 0                    ADDRESS TO BE SET
00223 -0 76000 0 00012          RTT
00224  0 76100 0 00000          NOP
00225  0 70000 0 00227  WTB8    CPY WTB10
00226  1 00003 0 00225  WTB9    TXI WTB8,0,3
00227  0 00000 0 00000  WTB10   PZE                      READ-BACK COPIED HERE
00230  0 76600 0 00333          IOD
00231 -0 76000 0 00012          RTT
00232  0 02000 0 00234          TRA WTB11
00233  0 02000 4 00003          TRA 3,4
00234  0 76400 0 00200  WTB11   BST 0                    ADDRESS TO BE SET
00235  2 00001 1 00212          TIX WTB2,1,1
00236  0 00000 0 00211          HTR WTB1                 RTT FAILS 3 TIMES. START TO TRY AGAIN
00237  0 76600 0 00220  WTB12   WTB 0                    CONSTANT
00240  0 76400 0 00200  WTB13   BST 0                    CONSTANT
                                   SUBROUTINE TO READ RECORD FROM TAPE
00241  0 50000 4 00001  RTB     CLA 1,4
00242  0 40000 0 00267          ADD RTB7
00243  0 60100 0 00252          STO RTB3
00244  0 50000 4 00001          CLA 1,4
00245  0 40000 0 00270          ADD RTB8
00246  0 60100 0 00264          STO RTB6
00247 -0 53400 1 00262  RTB1    LXD RTB5,1
00250  0 50000 4 00002  RTB2    CLA 2,4
00251  0 73400 2 00000          PAX 0,2
00252  0 76200 0 00220  RTB3    RTB 0                    TO BE SET
00253 -0 76000 0 00012          RTT
00254  0 76100 0 00000          NOP
00255  0 70000 2 00000  RTB4    CPY 0,2
00256  1 77777 2 00255          TXI RTB4,2,-1
00257  0 02000 4 00003          TRA 3,4
00260  0 76600 0 00333          IOD
```

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```
00261 -0 76000 0 00012         RTT
00262  1 00003 0 00264  RTB5   TXI RTB6,0,3
00263  0 02000 4 00004         TRA 4,4
00264  0 76400 0 00200  RTB6   BST 0                    TO BE SET
00265  2 00001 1 00250         TIX RTB2,1,1
00266  0 00000 0 00247         HTR RTB1                 RTT FAILS 3 TIMES. START TO TRY AGAIN.
00267  0 76200 0 00220  RTB7   RTB 0                    CONSTANT
00270  0 76400 0 00200  RTB8   BST 0                    CONSTANT
                                   TAKE DUMP FROM TAPE AND START CYCLE
00271  0 07400 4 00241  KA     TSX RTB,4
00272  0 00000 0 00004         PZE U1
00273  0 00000 0 77323         PZE -START
00274  0 00000 0 00165         HTR RCD                  END OF FILE
00275  0 76200 0 00224         RTB U1
00276  0 07400 4 00241         TSX RTB,4
00277  0 00000 0 00004         PZE U1
00300  0 00000 0 00400         PZE -32512
00301  0 00000 0 00165         HTR RCD
00302  0 77200 0 00204         REW U1
00303  0 02000 0 00455         TRA START
                                   TAKE OR XLS3 FROM TAPE AND ENTER
00304  0 76200 0 00224  KB     RTB U1
00305  0 70000 0 00315         CPY KB2
00306  0 02000 0 00310         TRA KB1
00307  0 00000 0 00165         HTR RCD                  OR XLS3 NOT ON TAPE. USE CARDS.
00310  0 07400 4 00241  KB1    TSX RTB,4
00311  0 00000 0 00004         PZE U1
00312  0 00000 0 77323         PZE -START
00313  0 00000 0 00165         HTR RCD                  END OF FILE
00314  0 02000 0 00455         TRA START
00315  0 00000 0 00000  KB2    PZE                      DISCARD COPIED HERE
                                   TAKE OR XLS4 FROM TAPE AND ENTER
00316  0 76200 0 00224  KC     RTB U1
00317  0 07400 4 00241         TSX RTB,4
00320  0 00000 0 00004         PZE U1
00321  0 00000 0 77323         PZE -START
00322  0 00000 0 00165         HTR RCD                  END OF FILE
00323  0 02000 0 00455         TRA START
                                   TAKE OR XLS5 FROM TAPE AND ENTER
00324  0 76200 0 00224  KD     RTB U1
00325  0 07400 4 00241         TSX RTB,4
00326  0 00000 0 00004         PZE U1
00327  0 00000 0 77323         PZE -START
```

```
00330  0 00000 0 00165          HTR RCD                    END OF FILE
00331  0 02000 0 00455          TRA START
                                    TAKE OR XLS2 FROM TAPE AND ENTER SECOND TIME
00332  0 07400 4 00241  KE      TSX RTB,4
00333  0 00000 0 00005          PZE U3
00334  0 00000 0 77323          PZE -START
00335  0 00000 0 00165          HTR RCD                    END OF FILE
00336  0 02000 0 00456          TRA START+1
                                    GET BACK ON WITH NEW PARAMETER SELECTION CARDS
00337  0 77200 0 00205  KF      REW U3
00340  0 76200 0 00225  KF1     RTB U3
00341  0 70000 0 00352          CPY KF3
00342  0 02000 0 00340          TRA KF1
00343  0 02000 0 00345          TRA KF2
00344  0 02000 0 00340          TRA KF1
00345  0 07400 4 00241  KF2     TSX RTB,4
00346  0 00000 0 00005          PZE U3
00347  0 00000 0 77323          PZE -START
00350  0 00000 0 00165          HTR RCD                    OR-XLS2 IS NOT ON TAPE
00351  0 02000 0 00460          TRA START+3
00352  0 00000 0 00000  KF3     PZE                        DISCARDS COPIED HERE
                  00455  START  EQU 301
                  00000          END 0
```

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```
                                        OR-XLS1   SEGMENT FOR PRELIMINARY DATA PROCESSING
                  00004  U1     EQU 4                  INPUT TAPE NUMBER
                  00040  U2     EQU 32                 NO OF ENTRIES IN EACH TABLE
                  00005  U3     EQU 5                  BINARY OUTPUT TAPE
                  00003  U4     EQU 3                  BCD OUTPUT TAPE NUMBER
                  00144  RCD    EQU 100
                  00157  KG     EQU 111
                  00455         ORG 301
00455  0 02000 0 00461  START  TRA XA
00456  0 00000 0 00144         HTR RCD                NO ENTRY HERE
00457  0 02000 0 01404         TRA DUMP
00460  0 00000 0 00144         HTR RCD                NO ENTRY HERE
00461  0 76200 0 00321  XA     RCD
00462  0 07400 4 01542         TSX DBD1,4
00463  0 00000 0 03200         PZE T12
00464  0 00000 0 00461         HTR XA                 END OF FILE
00465  0 07400 4 01261         TSX IFF,4
00466  0 01217 0 03213         PZE T12+11,0,IT
00467  0 02000 0 00461         TRA XA
00470  0 76200 0 00321  XA1    RCD
00471  0 07400 4 01542         TSX DBD1,4
00472  0 00000 0 02257         PZE BUFFER
00473  0 00000 0 00144         HTR RCD                END OF FILE
00474  0 07400 4 01261         TSX IFF,4
00475  0 01214 0 02272         PZE BUFFER+11,0,IC
00476  0 02000 0 00470         TRA XA1
00477  0 07400 4 01752         TSX FILE,4
00500 -1 00155 0 03156         MON D1,0,109
00501 -2 01772 0 03157         MTW D2,0,1018
00502 -2 03607 0 03160         MTW D3,0,1927
00503 -2 05424 0 03161         MTW D4,0,2836
00504 -2 07241 0 03162         MTW D5,0,3745
00505 -2 11056 0 03163         MTW D6,0,4654
00506 -2 12673 0 03164         MTW D7,0,5563
00507  0 00000 0 00144         HTR RCD                ERROR RETURN FROM FILE
00510  0 50000 0 03156  XB     CLA D1
00511  0 10000 0 00554         TZE XC
00512  0 56000 0 03156         LDQ D1
00513  0 20000 0 01221         MPY C2
00514 -0 60000 0 03165         STQ T1
00515  0 50000 0 01222         CLA C3
00516  0 40000 0 03165         ADD T1
00517  0 62100 0 01121         STA XQ2
```

```
    00520  0 62100 0 01124        STA XQ3
    00521  0 40200 0 01203        SUB I1
    00522  0 62100 0 01120        STA XQ1
    00523  0 50000 0 03165        CLA T1
    00524  0 40200 0 01221        SUB C2
    00525  0 40000 0 01203        ADD I1
    00526  0 60100 0 03176        STO T10
    00527  0 53400 1 01202        LXA I0,1
    00530  0 53400 2 03165        LXA T1,2
    00531  0 76200 0 00321  XB1   RCD
    00532  0 07400 4 01542        TSX DBD1,4
    00533  0 00000 0 02257        PZE BUFFER
    00534  0 00000 0 00144        HTR RCD                 END OF FILE
    00535  0 07400 4 01261        TSX IFF,4
    00536  0 01215 0 02272        PZE BUFFER+11,0,IF
    00537  0 02000 0 00531        TRA XB1
    00540  0 07400 4 01752        TSX FILE,4
    00541 -2 00155 1 03371        MTW M8+100,1,109
    00542 -2 01772 1 03372        MTW M8+101,1,1018
    00543 -2 03607 1 03373        MTW M8+102,1,1927
    00544 -2 05424 1 03374        MTW M8+103,1,2836
    00545 -2 07241 1 03375        MTW M8+104,1,3745
    00546 -2 11056 1 03376        MTW M8+105,1,4654
    00547 -2 12673 1 03377        MTW M8+106,1,5563
    00550 -2 14507 1 03400        MTW M8+107,1,6471
    00551  0 00000 0 00144        HTR RCD                 ERROR RETURN FROM FILE
    00552 -2 00010 2 00554        TNX XC,2,8
    00553  1 77770 1 00531        TXI XB1,1,-8
    00554  0 77200 0 00205  XC    REW U3
    00555  0 53400 4 01205        LXA I4,4
    00556  0 76600 0 00225  XC1   WTB U3
    00557  0 70000 0 01202        CPY I0
    00560  2 00001 4 00556        TIX XC1,4,1
    00561  0 76600 0 00333        IOD
    00562  0 76000 0 00162  XAA   SWT 2
TD  00563  1 00000 0 00565        TXI XBB
TD  00564  1 00000 0 00635        TXI XD
    00565  0 53400 1 01202  XBB   LXA I0,1
    00566  0 53400 2 03156        LXA D1,2
    00567 -3 00000 2 00577        TXL XBB4,2,0
    00570 -3 00013 2 00572        TXL XBB1,2,11
    00571  0 53400 2 01212        LXA I11,2
    00572  0 50000 0 01230  XBB1  CLA C14
```

```
        00573  0 60100 1 01160  XBB2   STO XT1,1
        00574  0 40200 0 01231         SUB C15
        00575  1 77777 1 00576         TXI XBB3,1,-1
        00576  2 00001 2 00573  XBB3   TIX XBB2,2,1
        00577  0 50000 0 01232  XBB4   CLA C16
        00600  0 60100 1 01160         STO XT1,1
        00601  0 50000 0 01233         CLA C17
        00602  0 60100 1 01161         STO XT1+1,1
        00603  0 07400 4 02326  XCC    TSX OUT,4
        00604  0 07400 4 01505         TSX ECHO,4
        00605  3 27451 0 03200         PTH T12,0,12073
        00606  3 02066 0 01220         PTH C1,0,1078
        00607  1 00001 0 00003         PON U4,0,1
        00610  0 07400 4 02326         TSX OUT,4
        00611  0 07400 4 01505         TSX ECHO,4
        00612  3 13625 0 01234         PTH C18,0,6037
        00613  1 00000 0 00003         PON U4,0,0
        00614  0 07400 4 02326         TSX OUT,4
        00615  0 07400 4 01505         TSX ECHO,4
        00616  3 05713 0 01242         PTH C19,0,3019
        00617 -3 15564 0 03157         SVN D2,0,7028
        00620 -3 15576 0 03160         SVN D3,0,7038
        00621 -3 15610 0 03161         SVN D4,0,7048
        00622 -3 15622 0 03162         SVN D5,0,7058
        00623 -3 15634 0 03163         SVN D6,0,7068
        00624 -3 15646 0 03164         SVN D7,0,7078
        00625  1 00000 0 00003         PON U4,0,0
        00626  0 07400 4 02326         TSX OUT,4
        00627  0 07400 4 01505         TSX ECHO,4
        00630  3 23516 0 01245         PTH C21,0,10062
        00631  1 00000 0 00003         PON U4,0,0
        00632  0 07400 4 02326         TSX OUT,4
        00633  0 07400 4 01505         TSX ECHO,4
        00634  1 00060 0 00003         PON U4,0,48
        00635  0 76000 0 00161  XD     SWT 1
TD      00636  1 00000 0 00652         TXI XF
        00637  0 76200 0 00321  XE     RCD
        00640  0 07400 4 01542         TSX DBD1,4
        00641  0 00000 0 02257         PZE BUFFER
        00642  0 02000 0 01176         TRA XV
        00643  0 07400 4 01261         TSX IFF,4
        00644  0 01216 0 02272         PZE BUFFER+11,0,IR
        00645  0 02000 0 00637         TRA XE
```

```
      00646  0 07400 4 01366          TSX BLNK,4
      00647  0 00011 0 02270          PZE BUFFER+9,0,9
      00650  0 02000 0 01176          TRA XV
      00651  0 02000 0 00677          TRA XEF
      00652  0 53400 1 01204  XF      LXA I3,1
      00653  0 76200 0 00204  XF1     RTD U1
      00654  0 53400 2 01213          LXA I14,2
      00655  0 70000 2 02275  XF2     CPY BUFFER+14,2
TD    00656  1 00000 0 00660          TXI XF3
TD    00657  1 00000 0 01175          TXI XU
      00660  2 00001 2 00655  XF3     TIX XF2,2,1
      00661  0 76600 0 00333          IOD
      00662 -0 76000 0 00012          RTT
TD    00663  1 00000 0 00665          TXI XF4
      00664  0 02000 0 00671          TRA XF5
      00665  0 76400 0 00204  XF4     BST U1
      00666  2 00001 1 00653          TIX XF1,1,1
      00667  0 76200 0 00204          RTD U1
      00670  0 00000 0 00652          HTR XF                  RTT FAILS 3 TIMES. START TO SKIP RECORD
      00671  0 07400 4 01261  XF5     TSX IFF,4
      00672  0 01216 0 02272          PZE BUFFER+11,0,IR
      00673  0 00000 0 00144          HTR RCD                 INCORRECT SYMBOL WAS ON TAPE
      00674  0 07400 4 01366          TSX BLNK,4
      00675  0 00013 0 02272          PZE BUFFER+11,0,11
      00676  0 02000 0 01175          TRA XU
      00677  0 07400 4 01752  XEF     TSX FILE,4
      00700 -2 00155 0 03216          MTW M1,0,109
      00701 -2 01772 0 03217          MTW M2,0,1018
      00702 -2 03607 0 03220          MTW M3,0,1927
      00703 -2 05424 0 03221          MTW M4,0,2836
      00704 -2 07241 0 03222          MTW M5,0,3745
      00705 -1 11056 0 03223          MON M6,0,4654
      00706 -2 12673 0 03214          MTW T13,0,5563
      00707 -2 14507 0 03215          MTW T14,0,6471
      00710  0 00000 0 00144          HTR RCD                 ERROR RETURN FROM FILE
      00711  0 14000 0 00712  XG      TQV XG1
      00712  0 16100 0 00713  XG1     TQO XG2
      00713  0 53400 1 01204  XG2     LXA I3,1
      00714  0 56000 1 03162  XG3     LDQ D5,1
      00715  0 26000 1 03221          FMP M4,1
      00716  0 60100 1 03171          STO T5,1
      00717  2 00001 1 00714          TIX XG3,1,1
      00720  0 56000 0 03162          LDQ D5
```

```
      00721  0 26000 0 03167          FMP T3
      00722  0 76500 0 00043          LRS 35
      00723  0 26000 0 03170          FMP T4
      00724  0 60100 0 03171          STO T5
      00725  0 56000 0 03163          LDQ D6
      00726  0 26000 0 03166          FMP T2
      00727  0 76500 0 00043          LRS 35
      00730  0 26000 0 03170          FMP T4
      00731  0 30000 0 03171          FAD T5
      00732  0 60100 0 03171          STO T5
      00733  0 56000 0 03164          LDQ D7
      00734  0 26000 0 03166          FMP T2
      00735  0 76500 0 00043          LRS 35
      00736  0 26000 0 03167          FMP T3
      00737  0 30000 0 03171          FAD T5
      00740  0 60100 0 03171          STO T5
      00741  0 30000 0 03171          FAD T5
      00742  0 60100 0 03171          STO T5
      00743  0 53400 1 01204          LXA I3,1
      00744  0 56000 1 03171  XG4     LDQ T5,1
      00745  0 26000 1 03171          FMP T5,1
      00746  0 30000 0 03171          FAD T5
      00747  0 60100 0 03171          STO T5
      00750  2 00001 1 00744          TIX XG4,1,1
      00751  0 56000 0 03171          LDQ T5
      00752  0 26000 0 01223          FMP C9
      00753  0 60100 0 03224          STO M7
      00754  0 16100 0 00756          TQO XG5
      00755 -0 14000 0 00757          TNO XH
      00756  0 00000 0 00144  XG5     HTR RCD              SIN THETA/LAMBDA SQUARED OVERFLOWS
      00757  0 02000 0 01060  XH      TRA XJ
                      00760  XI      BSS 64
      01060  0 50000 0 03222  XJ      CLA M5
      01061  0 60100 0 03172          STO T6
      01062  0 10000 0 01066          TZE XK
      01063  0 50000 0 01224          CLA C10
      01064  0 24000 0 03222          FDH M5
      01065 -0 60000 0 03222          STQ M5
      01066  0 50000 0 03223  XK      CLA M6
      01067 -0 10000 0 01073          TNZ XM
      01070  0 50000 0 03173  XL      CLA T7
      01071  0 60100 0 03223          STO M6
TD    01072  1 00000 0 01074          TXI XN
```

```
      01073  0 60100 0 03173  XM     STO T7
      01074  0 50000 0 03156  XN     CLA D1
      01075  0 10000 0 01130         TZE XR
      01076  0 50000 0 03224  XO     CLA M7
      01077  0 07400 4 02275         TSX SQRT,4
      01100  0 00000 0 00144         HTR RCD                NEGATIVE RADICAND
      01101  0 60100 0 03174         STO T8
      01102  0 56000 0 03174  XP     LDQ T8
      01103  0 26000 0 01227         FMP C13
      01104  0 60100 0 03175         STO T9
      01105 -0 30000 0 01225         UFA C11
      01106  0 73400 1 00000         PAX 0,1
      01107 -3 00037 1 01111         TXL XP1,1,U2-1
      01110  0 00000 0 00144         HTR RCD                OUT OF RANGE OF F TABLE
      01111  0 40000 0 03176  XP1    ADD T10
      01112  0 73400 1 00000         PAX 0,1
      01113 -0 60000 0 03177         STQ T11
      01114  0 50000 0 03177         CLA T11
      01115  0 30000 0 01226         FAD C12
      01116  0 60100 0 03177         STO T11
      01117  0 53400 2 01202  XQ     LXA I0,2
      01120  0 50000 1 00000  XQ1    CLA 0,1
      01121  0 30200 1 00000  XQ2    FSB 0,1
      01122  0 76500 0 00043         LRS 35
      01123  0 26000 0 03177         FMP T11
      01124  0 30000 1 00000  XQ3    FAD 0,1
      01125  0 60100 2 03225         STO M8,2
      01126  1 77777 2 01127         TXI XQ4,2,-1
      01127  2 00040 1 01120  XQ4    TIX XQ1,1,U2
      01130  0 76600 0 00225  XR     WTB U3
      01131  0 50000 0 03156         CLA D1
      01132  0 40000 0 01210         ADD I7
      01133  0 73400 1 00000         PAX 0,1
      01134  0 53400 2 01202         LXA I0,2
      01135  0 70000 2 03216  XR1    CPY M1,2
      01136  1 77777 2 01137         TXI XR2,2,-1
      01137  2 00001 1 01135  XR2    TIX XR1,1,1
      01140  0 70000 0 01202         CPY I0
      01141  0 70000 0 01202         CPY I0
      01142  0 76600 0 00333         IOD
      01143  0 76000 0 00162  XS     SWT 2
TD    01144  1 00000 0 01146         TXI XT
TD    01145  1 00000 0 00635         TXI XD
```

```
01146  0 07400 4 02326  XT    TSX OUT,4
01147  0 07400 4 01505        TSX ECHO,4
01150  3 03734 0 01257        PTH C22,0,2012
01151 -3 00004 0 03216        SVN M1,0,4
01152 -3 00010 0 03217        SVN M2,0,8
01153 -3 00014 0 03220        SVN M3,0,12
01154 -3 05716 0 03221        SVN M4,0,3022
01155 -3 05730 0 03172        SVN T6,0,3032
01156 -0 00043 0 03223        FOR M6,0,35
01157 -3 11663 0 03224        SVN M7,0,5043
                 01160  XT1   BSS 13
01175  0 77200 0 00204  XU    REW U1
01176  0 77000 0 00205  XV    WEF U3
01177  0 77000 0 00205        WEF U3
01200  0 77200 0 00205        REW U3
01201  0 02000 0 00157        TRA KG
                              CONSTANTS
01202  0 00000 0 00000  I0    PZE 0
01203  0 00000 0 00001  I1    PZE 1
01204  0 00000 0 00003  I3    PZE 3
01205  0 00000 0 00004  I4    PZE 4
01206  0 00000 0 00005  I5    PZE 5
01207  0 00000 0 00006  I6    PZE 6
01210  0 00000 0 00007  I7    PZE 7
01211  0 00000 0 00010  I8    PZE 8
01212  0 00000 0 00013  I11   PZE 11
01213  0 00000 0 00016  I14   PZE 14
01214  000000000023     IC    BCD 100000C
01215  000000000026     IF    BCD 100000F
01216  000000000051     IR    BCD 100000R
01217  000000000063     IT    BCD 100000T
01220  606060606060     C1    BCD 1
01221  0 00000 0 00040  C2    PZE U2                 NUMBER OF ENTRIES IN EACH F TABLE
01222  0 00000 0 03371  C3    PZE M8+100             ADDRESS OF FIRST F TABLE
01223 +177400000000     C9    DEC .25                FLOATING ONE QUARTER
01224 +201400000000     C10   DEC 1.                 FLOATING CONSTANT ONE
01225 +233000000000     C11   OCT 233000000000       FIXER TO GET INTEGER
01226 +200000000000     C12   OCT 200000000000       FIXER TO NORMALIZE FRACTION
01227 +205500000000     C13   DEC 20.                1/DELTA
01230 -3 05752 0 03225  C14   SVN M8,0,3050           INITIAL LINK WORDS FOR OUTPUT
01231  0 00007 0 00001  C15   PZE 1,0,7               CONSTANT TO ADVANCE LINK WORD
01232  1 00060 0 00003  C16   PON U4,0,48             TAPE WRITE ORDER
TD 01233  1 00000 0 00635  C17   TXI XD                TRANSFER AFTER OUTPUT
```

```
01234  314547646360      C18   BCD 6INPUT DATA AS PROCESSED BY OR-XLS1
01235  242163216021
01236  626047514623
01237  256262252460
01240  227060465140
01241  674362016060
01242  232543436023      C19   BCD 3CELL CONSTANTS
01243  464562632145
01244  636260606060
01245  603060606042      C21   BCD   H   K   L  OBSERVED    SIGMA   Q   RHO      FORM FACTORS
01246  606060436060
01247  462262255165
01250  252460606060
01251  623127442160
01252  606050606060
01253  513046606060
01254  606060264651
01255  446026212363
01256  465162606060
01257  606060006060      C22   BCD 2   0   0   0
01260  600060606000
                                   SUBROUTINE TO CHECK IDENTIFICATION LETTER
01261   0 76000 0 00166  IFF   SWT 6
01262   0 02000 0 01264        TRA IFF1
01263   0 02000 4 00003        TRA 3,4
01264   0 50000 4 00001  IFF1  CLA 1,4
01265   0 62100 0 01271        STA IFF2
01266   0 77100 0 00022        ARS 18
01267   0 62100 0 01274        STA IFF3
01270   0 62100 0 01307        STA IFF6
01271   0 50000 0 00000  IFF2  CLA 0                 ADDRESS TO BE SET
01272  -0 32000 0 01364        ANA IFF11
01273   0 60100 0 01365        STO IFF12
01274   0 34000 0 00000  IFF3  CAS 0                 ADDRESS TO BE SET
01275   1 00000 0 01277  IFF4  TXI IFF5,0,0
01276   0 02000 4 00003        TRA 3,4
01277  -0 63400 4 01275  IFF5  SXD IFF4,4
01300   0 07400 4 02326        TSX OUT,4
01301   0 07400 4 01505        TSX ECHO,4
01302   3 02015 0 01365        PTH IFF12,0,1037
01303   3 13624 0 01327        PTH IFF7,0,6036
01304  -1 00000 0 00364        FVE 244
01305   0 07400 4 02326        TSX OUT,4
```

```
01306  0 07400 4 01505          TSX ECHO,4
01307  3 02015 0 00000  IFF6    PTH 0,0,1037          ADDRESS TO BE SET
01310  3 13624 0 01335          PTH IFF8,0,6036
01311 -1 00000 0 00364          FVE 244
01312  0 07400 4 02326          TSX OUT,4
01313  0 07400 4 01505          TSX ECHO,4
01314  3 15602 0 01343          PTH IFF9,0,7042
01315 -1 00000 0 00364          FVE 244
01316  0 07400 4 02326          TSX OUT,4
01317  0 07400 4 01505          TSX ECHO,4
01320  3 23514 0 01352          PTH IFF10,0,10060
01321 -1 00000 0 00364          FVE 244
01322  0 07400 4 02326          TSX OUT,4
01323  0 07400 4 01505          TSX ECHO,4
01324 -1 00000 0 00361          FVE 241
01325 -0 53400 4 01275          LXD IFF4,4
01326  0 00000 4 00002          HTR 2,4
01327  602421632160      IFF7   BCD 6 DATA CARD IDENTIFICATION LETTER IS
01330  232151246031
01331  242545633126
01332  312321633146
01333  456043256363
01334  255160316260
01335  604751462751      IFF8   BCD 6 PROGRAM CALLS FOR CARD WITH LETTER
01336  214460232143
01337  436260264651
01340  602321512460
01341  663163306043
01342  256363255160
01343  604764636023      IFF9   BCD 7 PUT CORRECT CARD IN READER AND PROCEED.
01344  465151252363
01345  602321512460
01346  314560512521
01347  242551602145
01350  246047514623
01351  252524336060
01352  606346602270      IFF10  BCD   TO BYPASS ALL IDENTIFICATION TESTS TURN ON SENSE SWITCH 6.
01353  472162626021
01354  434360312425
01355  456331263123
01356  216331464560
01357  632562636260
01360  636451456046
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01361  456062254562
01362  256062663163
01363  233060063360
01364   0 00000 0 00177  IFF11 PZE 127                    MASK
01365   0 00000 0 00000  IFF12                            LETTER FROM CARD
                                 SUBROUTINE TO TEST FOR BLANK FIELD
01366  -0 63400 1 01374  BLNK  SXD BLNK2,1
01367   0 50000 4 00001         CLA 1,4
01370   0 62100 0 01372         STA BLNK1
01371  -0 73400 1 00000         PDX 0,1
01372   0 50000 1 00000  BLNK1 CLA 0,1                    ADDRESS TO BE SET
01373   0 34000 0 01403         CAS BLNK5
01374   1 00000 0 01376  BLNK2 TXI BLNK3,0,0
01375   0 02000 0 01400         TRA BLNK4
01376  -0 53400 1 01374  BLNK3 LXD BLNK2,1
01377   0 02000 4 00003         TRA 3,4
01400   2 00001 1 01372  BLNK4 TIX BLNK1,1,1
01401  -0 53400 1 01374         LXD BLNK2,1
01402   0 02000 4 00002         TRA 2,4
01403   606060606060     BLNK5 BCD 1
                                 OCTAL AND FLOATING DECIMAL DUMP FOR TEST PURPOSES
01404   0 07400 4 02326  DUMP  TSX OUT,4
01405   0 07400 4 01505         TSX ECHO,4
01406   3 27451 0 03200         PTH T12,0,12073
01407   3 02066 0 01220         PTH C1,0,1078
01410   1 00001 0 00003         PON U4,0,1
01411   0 53400 1 01503         LXA DUMP7,1
01412   0 07400 4 02326  DUMP1 TSX OUT,4
01413   0 07400 4 01505         TSX ECHO,4
01414  -2 17531 1 00000         SIX 0,1,8025
01415  -2 17562 1 00001         SIX 1,1,8050
01416  -2 17613 1 00002         SIX 2,1,8075
01417  -2 17644 1 00003         SIX 3,1,8100
01420   1 00000 0 00003         PON U4,0,0
01421  -0 75400 1 00000         PXD 0,1
01422   0 77100 0 00022         ARS 18
01423   0 76000 0 00006         COM
01424   0 40000 0 01203         ADD I1
01425   0 73400 2 00000         PAX 0,2
01426  -0 75400 2 00000         PXD 0,2
01427   0 76500 0 00043         LRS 35
01430   0 53400 4 01207         LXA I6,4
01431   0 76700 0 00003  DUMP8 ALS 3
```

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01432 -0 76300 0 00003          LGL 3
01433  2 00001 4 01431          TIX DUMP8,4,1
01434 -0 50100 0 01504          ORA DUMP9
01435  0 60200 0 01502          SLW DUMP6+8
01436  0 53400 2 01211          LXA I8,2
01437  0 56000 1 00000  DUMP2   LDQ 0,1
01440  0 53400 4 01207          LXA I6,4
01441  0 76700 0 00003  DUMP3   ALS 3
01442 -0 76300 0 00003          LGL 3
01443  2 00001 4 01441          TIX DUMP3,4,1
01444  0 60200 2 01502          SLW DUMP6+8,2
01445  0 53400 4 01207          LXA I6,4
01446  0 76700 0 00003  DUMP4   ALS 3
01447 -0 76300 0 00003          LGL 3
01450  2 00001 4 01446          TIX DUMP4,4,1
01451  0 60200 2 01503          SLW DUMP6+9,2
01452  1 77777 1 01453          TXI DUMP5,1,-1
01453  2 00002 2 01437  DUMP5   TIX DUMP2,2,2
01454  0 07400 4 02326          TSX OUT,4
01455  0 07400 4 01505          TSX ECHO,4
01456  3 01756 0 01502          PTH DUMP6+8,0,1006
01457  3 01772 0 01472          PTH DUMP6,0,1018
01460  3 02001 0 01473          PTH DUMP6+1,0,1025
01461  3 02023 0 01474          PTH DUMP6+2,0,1043
01462  3 02032 0 01475          PTH DUMP6+3,0,1050
01463  3 02054 0 01476          PTH DUMP6+4,0,1068
01464  3 02063 0 01477          PTH DUMP6+5,0,1075
01465  3 02105 0 01500          PTH DUMP6+6,0,1093
01466  3 02114 0 01501          PTH DUMP6+7,0,1100
01467  1 00060 0 00003          PON U4,0,48
01470  3 74541 1 01412          TXH DUMP1,1,-M8-10    DECREMENT IS -(FINAL ADDRESS+1)
01471  0 02000 0 00144          TRA RCD
                 01472  DUMP6   BSS 9
01503  0 00000 0 74622  DUMP7   PZE -D1               -(INITIAL ADDRESS)
01504  600000000000     DUMP9   BCD 1 00000
                                     SUBROUTINE TO TEST NATURE OF ERROR RETURN FROM NY OUT3
01505  0 12000 0 01523  ECHO    TPL ECHO4
01506 -0 10000 0 01523          TNZ ECHO4
01507 -0 63400 4 01541          SXD ECHO7,4
01510  0 07400 4 02326          TSX OUT,4
01511  0 02000 0 01514          TRA ECHO2
01512  3 15602 0 01532          PTH ECHO6,0,7042
01513 -1 00000 0 00000  ECHO1   FVE
```

```
01514 -0 53400 4 01541  ECHO2 LXD ECHO7,4
01515 -0 50000 4 00001  ECHO3 CAL 1,4
01516  0 77100 0 00041        ARS 33
01517  0 34000 0 01531        CAS ECHO5
01520  1 77777 4 01515        TXI ECHO3,4,-1
01521  0 02000 4 00002        TRA 2,4                 TO NORMAL RETURN OF NY OUT3
01522  1 77777 4 01515        TXI ECHO3,4,-1
01523 -0 75400 4 00000  ECHO4 PXD 0,4
01524  0 76000 0 00006        COM
01525 -0 73400 4 00000        PDX 0,4
01526 -0 75400 4 00000        PXD 0,4
01527  0 77100 0 00022        ARS 18
01530  0 00000 0 00144        HTR RCD                 CALLING SEQUENCE ERROR. ADDRESS IN ACC.
01531  0 00000 0 00005  ECHO5 FZE 5
01532  605454546047     ECHO6 BCD 7 *** PRINTER ERROR IN PREVIOUS LINE ***
01533  513145632551
01534  602551514651
01535  603145604751
01536  256531466462
01537  604331452560
01540  545454606060
01541  0 00000 0 00000  ECHO7 PZE                     INDEX SAVED IN DECREMENT
                                THE FOLLOWING SUBROUTINES ARE ON RELOCATABLE CARDS
                 01542  DBD1   BSS 136
                 01752  FILE   BSS 197
                 02257 BUFFER  BSS 14
                 02275  SQRT   BSS 25
                 02326  OUT    BSS 408
                                DATA STORAGE
03156  0 00000 0 00000  D1                            NUMBER OF FORM FACTOR TABLES
03157  0 00000 0 00000  D2                            A*
03160  0 00000 0 00000  D3                            B*
03161  0 00000 0 00000  D4                            C*
03162  0 00000 0 00000  D5                            COS ALPHA*
03163  0 00000 0 00000  D6                            COS BETA*
03164  0 00000 0 00000  D7                            COS GAMMA*
                                TEMPORARY STORAGE
03165  0 00000 0 00000  T1                            TOTAL NO OF ENTRIES IN TABLES
03166  0 00000 0 00000  T2                            HA*
03167  0 00000 0 00000  T3                            KB*
03170  0 00000 0 00000  T4                            LC*
03171  0 00000 0 00000  T5                            4(SIN THETA/LAMBDA)**2=Q
03172  0 00000 0 00000  T6                            SIGMA FOR BCD OUTPUT
```

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```
03173  0 00000 0 00000  T7                          CURRENT VALUE OF S. SEE M6
03174  0 00000 0 00000  T8                          SIN THETA/LAMBDA
03175  0 00000 0 00000  T9                          (SIN THETA/LAMBDA)(1/DELTA)
03176  0 00000 0 00000  T10                         (U2)(D1-1)+1
03177  0 00000 0 00000  T11                         FRACTIONAL PART OF T9
                 03200  T12   BSS 12                OUTPUT HEADING
03214  0 00000 0 00000  T13                         EXTRA INPUT 1
03215  0 00000 0 00000  T14                         EXTRA INPUT 2
                                STORAGE FOR BINARY OUTPUT
03216  0 00000 0 00000  M1                          H
03217  0 00000 0 00000  M2                          K
03220  0 00000 0 00000  M3                          L
03221  0 00000 0 00000  M4                          OBSERVED F OR F SQUARED
03222  0 00000 0 00000  M5                          1/SIGMA=SQRT OF WEIGHT
03223  0 00000 0 00000  M6                          S, SCALE FACTOR DESIGNATION
03224  0 00000 0 00000  M7                          (SIN THETA/LAMBDA)**2=Q/4
03225  0 00000 0 00000  M8                          COMPUTED FORM FACTORS
                                THIS SECTION SUPPLIES ORIGIN CARDS FOR THE SUBROUTINES
                 00000        ORG 0
00000  0 00000 0 00000        PZE
00001  0 00000 0 01542        PZE DBD1
                 00000        ORG 0
00000  0 00000 0 00000        PZE
00001  0 00000 0 01752        PZE FILE
                 00000        ORG 0
00000  0 00000 0 00000        PZE
00001  0 00000 0 02275        PZE SQRT
                 00000        ORG 0
00000  0 00000 0 00000        PZE
00001  0 00000 0 02326        PZE OUT
                 00000        END 0
```

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                    00144  RCD    EQU 100
                    00145  LDCD   EQU 101
                    00146  WTB    EQU 102
                    00160  KH     EQU 112
                    00161  KI     EQU 113
                    00004  U1     EQU 4                  NUMBER OF BINARY INPUT TAPE
                    00003  U2     EQU 3                  NUMBER OF BCD OUTPUT TAPE
                    00005  U3     EQU 5                  NUMBER OF BINARY OUTPUT TAPE
                    00455         ORG 301
00455   0 02000 0 00461  START TRA XCA
00456   0 02000 0 03334         TRA XTD
00457   0 02000 0 05153         TRA DUMP
00460   0 02000 0 03164         TRA XSB
00461   0 76200 0 00321  XCA    RCD
00462   0 07400 4 05363         TSX DBD1,4
00463   0 00000 0 10406         PZE T55
00464   0 00000 0 00144         HTR RCD                END OF FILE
00465   0 07400 4 05030         TSX IFF,4
00466   0 04357 0 10421         PZE T55+11,0,IT
00467   0 02000 0 00461         TRA XCA
00470   0 02000 0 02250  XCB    TRA XDA
00471   0 02000 0 02712  XCC    TRA XEB
00472   0 53400 1 10324  XRA    LXA T61,1              OR TXI XCD
00473   0 53400 2 10316         LXA S10,2
00474   0 76200 0 00321  XRB    RCD
00475   0 07400 4 05363         TSX DBD1,4
00476   0 00000 0 06100         PZE BUFFER
00477   0 00000 0 00144         HTR RCD                END OF FILE
00500   0 07400 4 05030         TSX IFF,4
00501   0 04354 0 06113         PZE BUFFER+11,0,IM
00502   0 02000 0 00474         TRA XRB
00503   0 07400 4 05135         TSX BLNK,4
00504   0 00010 0 06110         PZE BUFFER+8,0,8
00505   0 02000 0 00550         TRA XRI
00506   0 07400 4 05573  XRC    TSX FILE,4
00507  -2 00157 1 00000         MTW 0,1,111
00510  -2 03132 1 00002         MTW 2,1,1626
00511  -2 06105 1 00004         MTW 4,1,3141
00512  -0 01455 0 10435         MZE T63,0,813
00513  -0 04430 0 10436         MZE T63+1,0,2328
00514  -0 07403 0 10437         MZE T63+2,0,3843
00515  -0 01767 0 10440         MZE T63+3,0,1015
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00516 -0 04742 0 10441          MZE T63+4,0,2530
00517 -0 07715 0 10442          MZE T63+5,0,4045
00520  0 00000 0 00144          HTR RCD                 ERROR RETURN FROM FILE
00521  0 53400 4 04340  XRD     LXA I3,4
00522  0 50000 0 04634  XRE     CLA C60
00523 -0 32000 4 10440          ANA T63+3,4
00524  0 10000 0 00532          TZE XRE1
00525  0 40200 0 04340          SUB I3
00526  0 56000 4 10440          LDQ T63+3,4
00527 -0 77300 0 00031          RQL 25
00530  0 16200 0 00532          TQP XRE1
00531  0 40200 0 04340          SUB I3
00532  0 76700 0 00022  XRE1    ALS 18
00533  0 60100 1 00001          STO 1,1
00534  0 50000 0 04634          CLA C60
00535 -0 32000 4 10443          ANA T63+6,4
00536  0 10000 0 00544          TZE XRE2
00537  0 40200 0 04340          SUB I3
00540  0 56000 4 10443          LDQ T63+6,4
00541 -0 77300 0 00031          RQL 25
00542  0 16200 0 00544          TQP XRE2
00543  0 40200 0 04340          SUB I3
00544 -0 60200 1 00001  XRE2    ORS 1,1
00545  1 77776 1 00546  XRF     TXI XRG,1,-2
00546  2 00001 4 00522  XRG     TIX XRE,4,1
00547  2 00001 2 00474  XRH     TIX XRB,2,1
00550  0 76200 0 00321  XRI     RCD
00551  0 07400 4 05363          TSX DBD1,4
00552  0 00000 0 06100          PZE BUFFER
00553  0 00000 0 00144          HTR RCD                 END OF FILE
00554  0 07400 4 05030          TSX IFF,4
00555  0 04352 0 06113          PZE BUFFER+11,0,IC
00556  0 02000 0 00550          TRA XRI
00557  0 07400 4 05135          TSX BLNK,4
00560  0 00013 0 06113          PZE BUFFER+11,0,11
00561  0 02000 0 00620          TRA XCD
00562  0 07400 4 05573          TSX FILE,4
00563 -2 01772 0 10462          MTW T78,0,1018
00564 -2 03607 0 10463          MTW T79,0,1927
00565 -2 05424 0 10464          MTW T80,0,2836
00566 -2 07241 0 10467          MTW T83,0,3745
00567 -2 11056 0 10466          MTW T82,0,4654
00570 -2 12673 0 10465          MTW T81,0,5563
```

```
00571  0 00000 0 00144        HTR RCD          ERROR RETURN FROM FILE
00572  0 56000 0 10462  XRJ   LDQ T78
00573  0 26000 0 10463        FMP T79
00574  0 60100 0 10473        STO T87
00575  0 56000 0 10462        LDQ T78
00576  0 26000 0 10464        FMP T80
00577  0 60100 0 10474        STO T88
00600  0 56000 0 10463        LDQ T79
00601  0 26000 0 10464        FMP T80
00602  0 60100 0 10475        STO T89
00603  0 53400 1 04340        LXA I3,1
00604  0 56000 1 10465  XRJ1  LDQ T78+3,1
00605  0 26000 1 10465        FMP T78+3,1
00606  0 60100 1 10473        STO T84+3,1
00607  0 56000 1 10476        LDQ T87+3,1
00610  0 26000 1 10470        FMP T81+3,1
00611  0 60100 1 10476        STO T87+3,1
00612  2 00001 1 00604        TIX XRJ1,1,1
00613  0 53400 1 04343        LXA I6,1
00614  0 56000 0 04752  XRJ2  LDQ C80
00615  0 26000 1 10476        FMP T84+6,1
00616  0 60100 1 10476        STO T84+6,1
00617  2 00001 1 00614        TIX XRJ2,1,1
00620  0 02000 0 03034  XCD   TRA XFB
00621  0 77200 0 00204  XCE   REW U1
00622  0 53400 4 04341        LXA I4,4
00623  0 76200 0 00224  XCE1  RTB U1
00624  0 70000 0 10450        CPY T69
00625  0 02000 0 00627        TRA XCE2
00626  0 00000 0 00144        HTR RCD          END OF FILE
00627  2 00001 4 00623  XCE2  TIX XCE1,4,1
00630  0 50000 0 05025  XCF   CLA C90          OR TRA XCG
00631  0 40200 0 10330        SUB T11
00632  0 77100 0 00001        ARS 1
00633  0 60100 0 10504        STO T96
00634  0 77100 0 00001        ARS 1
00635  0 40000 0 10504        ADD T96
00636  0 73400 1 00000        PAX 0,1
00637  0 77200 0 00205        REW U3
00640  0 76600 0 00225        WTB U3
00641  0 70000 0 04335  XCF1  CPY I0
00642  2 00001 1 00641        TIX XCF1,1,1
00643  0 53400 1 10504        LXA T96,1
```

```
00644  0 76600 0 00225        WTB U3
00645  0 70000 0 04335  XCF2  CPY I0
00646  2 00001 1 00645        TIX XCF2,1,1
00647  0 53400 1 05026        LXA C91,1
00650  0 76600 0 00225        WTB U3
00651  0 70000 0 04335  XCF3  CPY I0
00652  2 00001 1 00651        TIX XCF3,1,1
00653  0 53400 1 05027        LXA C92,1
00654  0 76600 0 00225        WTB U3
00655  0 70000 0 04335  XCF4  CPY I0
00656  2 00001 1 00655        TIX XCF4,1,1
00657  0 76600 0 00333        IOD
00660  0 53400 1 04343  XCG   LXA I6,1
00661  0 60000 1 10377  XCG1  STZ T42+6,1
00662  2 00001 1 00661        TIX XCG1,1,1
00663  0 60000 0 10444        STZ T65
00664  0 60000 0 10445        STZ T66
00665  0 60000 0 10500        STZ T92
00666  0 60000 0 05362  XCH   STZ SWTF8              OR TRA XA
00667  0 76000 0 00163        SWT 3
00670  0 02000 0 00672        TRA XCH1
00671  0 02000 0 00700        TRA XCH2
00672  0 07400 4 06147  XCH1  TSX OUT,4
00673  0 07400 4 05254        TSX ECHO,4
00674  3 23514 0 05005        PTH C86,0,10060
00675  3 06002 0 05021        PTH C88,0,3074
00676 -0 00027 0 04340        FOR I3,0,23
00677 -1 00000 0 00364        FVE 244
00700  0 07400 4 05336  XCH2  TSX SWTF,4
00701  0 00000 0 00707        PZE XCH3
00702  0 07400 4 06147        TSX OUT,4
00703  0 07400 4 05254        TSX ECHO,4
00704  3 27451 0 10406        PTH T55,0,12073
00705  3 02066 0 04362        PTH C3,0,1078
00706  1 00001 0 00003        PON U2,0,1
00707 -1 00000 0 00364  XCH3  FVE 244
00710  0 07400 4 05336  XCH4  TSX SWTF,4
00711  0 00000 0 00716        PZE XCH6
00712  0 07400 4 06147        TSX OUT,4
00713  0 07400 4 05254        TSX ECHO,4
00714  0 00000 0 00000  XCH5  PZE                    TO BE SET
00715  1 00000 0 00003        PON U2,0,0
00716 -1 00000 0 00364  XCH6  FVE 244
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     00717  0 07400 4 05336  XCH7   TSX SWTF,4
     00720  0 00000 0 00724         PZE XCH8
     00721  0 07400 4 06147         TSX OUT,4
     00722  0 07400 4 05254         TSX ECHO,4
     00723  1 00060 0 00003         PON U2,0,48
     00724 -1 00000 0 00000  XCH8   FVE
     00725  0 53400 4 04340  XA     LXA I3,4
     00726  0 76200 0 00224  XA1    RTB U1
     00727 -0 76000 0 00012         RTT
     00730  0 76100 0 00000         NOP
     00731  0 53400 1 04344         LXA I7,1
     00732  0 70000 1 10514  XA2    CPY M1+7,1
TD   00733  1 00000 0 00736         TXI XA3
TD   00734  1 00000 0 02065         TXI XBI
     00735  0 00000 0 00144         HTR RCD                RECORD TOO SHORT
     00736  2 00001 1 00732  XA3    TIX XA2,1,1
     00737  0 53400 1 10313         LXA T4,1
     00740 -3 00000 1 00746         TXL XA5,1,0
     00741  0 53400 2 10330         LXA T11,2
     00742  0 70000 2 00000  XA4    CPY 0,2
     00743 -2 00001 1 00746         TNX XA5,1,1
     00744  1 77777 2 00742         TXI XA4,2,-1
     00745  0 00000 0 00144         HTR RCD                RECORD TOO SHORT
     00746  0 53400 1 04346  XA5    LXA I9,1
     00747  0 70000 1 10525  XA6    CPY M8+9,1
     00750  2 00001 1 00747         TIX XA6,1,1
TD   00751  1 00000 0 00753         TXI XA7
TD   00752  1 00000 0 00757         TXI XA9
     00753  0 53400 1 10327  XA7    LXA T8,1
     00754  0 70000 1 00000  XA8    CPY 0,1
     00755  1 77777 1 00754         TXI XA8,1,-1
     00756  0 00000 0 00000         PZE
     00757  0 76600 0 00333  XA9    IOD
     00760 -0 76000 0 00012         RTT
TD   00761  1 00000 0 00763         TXI XA10
TD   00762  1 00000 0 00767         TXI XB
     00763  0 76400 0 00204  XA10   BST U1
     00764  2 00001 4 00726         TIX XA1,4,1
     00765  0 76200 0 00224         RTB U1
     00766  0 00000 0 00725         HTR XA                 RTT FAILS 3 TIMES. START TO SKIP RECORD
     00767  0 53400 1 10332  XB     LXA T10,1
     00770  0 53400 2 10326         LXA T7,2
     00771  0 60000 2 00000  XB1    STZ 0,2
```

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00772 -2 00001 1 00774          TNX XC,1,1
00773  1 77777 2 00771          TXI XB1,2,-1
00774  0 53400 4 10316  XC      LXA T1,4
00775  0 53400 1 10324          LXA T61,1
00776 -0 63400 1 10434          SXD T62,1
00777  0 76100 0 00000  XD      NOP                      OR TRA XD1
01000 -0 63400 4 10353  XE      SXD T28,4
01001  0 60000 0 10333  XF      STZ T12                  OR TRA XH
01002  0 53400 4 04343          LXA I6,4
01003  0 60000 4 10434  XF1     STZ T60+6,4
01004  2 00001 4 01003          TIX XF1,4,1
01005  0 53400 1 04340          LXA I3,1
01006 -0 53400 2 10434          LXD T62,2
01007  0 56000 1 10510  XF2     LDQ M1+3,1
01010  0 26000 2 00000          FMP 0,2
01011  0 30000 0 10333          FAD T12
01012  0 60100 0 10333          STO T12
01013  0 50000 2 00001          CLA 1,2
01014 -0 73400 4 00000          PDX 0,4
01015 -3 00000 4 01021          TXL XF3,4,0
01016  0 50000 1 10510          CLA M1+3,1
01017  0 30000 4 10434          FAD T60+6,4
01020  0 60100 4 10434          STO T60+6,4
01021  0 50000 2 00001  XF3     CLA 1,2
01022  0 73400 4 00000          PAX 0,4
01023 -3 00000 4 01027          TXL XF4,4,0
01024  0 50000 1 10510          CLA M1+3,1
01025  0 30000 4 10434          FAD T60+6,4
01026  0 60100 4 10434          STO T60+6,4
01027  1 77776 2 01030  XF4     TXI XF5,2,-2
01030  2 00001 1 01007  XF5     TIX XF2,1,1
01031 -0 63400 2 10434          SXD T62,2
01032  0 53400 1 04340          LXA I3,1
01033  0 53400 2 04335          LXA I0,2
01034  0 50200 1 10431  XF6     CLS T60+3,1
01035  0 30000 1 10434          FAD T60+6,1
01036  0 60100 2 10336          STO T15,2
01037  1 00001 2 01040          TXI XF7,2,1
01040  2 00001 1 01034  XF7     TIX XF6,1,1
TD     01041  1 00000 0 01070  XG      TXI XH                   OR LXA I3,1
01042  0 56000 1 10337  XG1     LDQ T13+3,1
01043  0 26000 1 10337          FMP T13+3,1
01044  0 60100 1 10342          STO T16+3,1
```

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01045  2 00001 1 01042          TIX XG1,1,1
01046  0 56000 0 10334          LDQ T13
01047  0 26000 0 10335          FMP T14
01050  0 60100 0 10342          STO T19
01051  0 56000 0 10342          LDQ T19
01052  0 26000 0 04366          FMP C7
01053  0 60100 0 10342          STO T19
01054  0 56000 0 10334          LDQ T13
01055  0 26000 0 10336          FMP T15
01056  0 60100 0 10343          STO T20
01057  0 56000 0 10343          LDQ T20
01060  0 26000 0 04366          FMP C7
01061  0 60100 0 10343          STO T20
01062  0 56000 0 10335          LDQ T14
01063  0 26000 0 10336          FMP T15
01064  0 60100 0 10344          STO T21
01065  0 56000 0 10344          LDQ T21
01066  0 26000 0 04366          FMP C7
01067  0 60100 0 10344          STO T21
01070  0 53400 4 10314  XH      LXA T2,4
01071  0 53400 2 10325          LXA T6,2
01072  0 53400 1 10326          LXA T7,1
01073  0 76100 0 00000  XI      NOP                    INSERT TRANSFER TO HANDLE SPECIAL POSITIONS
01074 -0 63400 4 10346          SXD T23,4
01075  0 50000 0 10333          CLA T12
01076  0 60100 0 10345          STO T22
01077  0 53400 4 04340          LXA I3,4
01100  1 77777 2 01101          TXI XI1,2,-1
01101  0 56000 2 00000  XI1     LDQ 0,2
01102  0 26000 4 10337          FMP T13+3,4
01103  0 30000 0 10345          FAD T22
01104  0 60100 0 10345          STO T22
01105  1 77777 2 01106          TXI XI2,2,-1
01106  2 00001 4 01101  XI2     TIX XI1,4,1
01107  0 07400 4 06777          TSX SIN,4
01110  0 60100 0 10347          STO T24
01111  0 50000 0 10345          CLA T22
01112  0 07400 4 07000          TSX SIN+1,4
01113  0 60100 0 10350          STO T25
01114  1 77777 2 01135  XJ      TXI XK,2,-1            OR LXA I6,4
01115  0 60000 0 10351          STZ T26
01116  0 56000 2 00000  XJ1     LDQ 0,2
01117  0 26000 4 10345          FMP T16+6,4
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        01120  0 30000 0 10351          FAD T26
        01121  0 60100 0 10351          STO T26
        01122  1 77777 2 01123          TXI XJ2,2,-1
        01123  2 00001 4 01116  XJ2     TIX XJ1,4,1
        01124  0 07400 4 07027          TSX EXP,4
        01125  0 00000 0 00144          HTR RCD                 NEGATIVE ANIS TEMP FACTOR
        01126  0 60100 0 10352          STO T27
        01127  0 56000 0 10352          LDQ T27
        01130  0 26000 0 10347          FMP T24
        01131  0 60100 0 10347          STO T24
        01132  0 56000 0 10352          LDQ T27
        01133  0 26000 0 10350          FMP T25
        01134  0 60100 0 10350          STO T25
        01135  0 50000 0 10350  XK      CLA T25
        01136  0 30000 1 00000          FAD 0,1
        01137  0 60100 1 00000          STO 0,1
        01140  1 77777 1 01141          TXI XL,1,-1
        01141  0 53400 4 04340  XL      LXA I3,4                OR TXI XN
        01142  0 56000 0 10347  XL1     LDQ T24
        01143  0 26000 4 10337          FMP T13+3,4
        01144  0 30000 1 00000          FAD 0,1
        01145  0 60100 1 00000          STO 0,1
        01146  1 77777 1 01147          TXI XL2,1,-1
        01147  2 00001 4 01142  XL2     TIX XL1,4,1
        01150  1 77777 1 01157  XM      TXI XN,1,-1             OR LXA I6,4
        01151  0 56000 0 10350  XM1     LDQ T25
        01152  0 26000 4 10345          FMP T16+6,4
        01153  0 30000 1 00000          FAD 0,1
        01154  0 60100 1 00000          STO 0,1
        01155  1 77777 1 01156          TXI XM2,1,-1
        01156  2 00001 4 01151  XM2     TIX XM1,4,1
TD      01157  1 00000 0 01201  XN      TXI XQ                  OR CLA T24
        01160  0 30000 1 00000          FAD 0,1
        01161  0 60100 1 00000          STO 0,1
        01162  1 77777 1 01163          TXI XO,1,-1
        01163  0 53400 4 04340  XO      LXA I3,4                OR TXI XQ
        01164  0 56000 0 10350  XO1     LDQ T25
        01165  0 26000 4 10337          FMP T13+3,4
        01166  0 30000 1 00000          FAD 0,1
        01167  0 60100 1 00000          STO 0,1
        01170  1 77777 1 01171          TXI XO2,1,-1
        01171  2 00001 4 01164  XO2     TIX XO1,4,1
        01172  1 77777 1 01201  XP      TXI XQ,1,-1             OR LXA I6,4
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01173  0 56000 0 10347  XP1   LDQ T24
01174  0 26000 4 10345        FMP T16+6,4
01175  0 30000 1 00000        FAD 0,1
01176  0 60100 1 00000        STO 0,1
01177  1 77777 1 01200        TXI XP2,1,-1
01200  2 00001 4 01173  XP2   TIX XP1,4,1
01201 -0 53400 4 10346  XQ    LXD T23,4
01202  2 00001 4 01073        TIX XI,4,1
01203 -0 53400 4 10353  XR    LXD T28,4
01204  2 00001 4 00777        TIX XD,4,1
01205  0 53400 4 10314  XS    LXA T2,4
01206  0 53400 2 10325        LXA T6,2
01207  0 53400 1 10326        LXA T7,1
01210  0 50000 0 04335  XS1   CLA I0                 OR TRA XS2
01211  0 56000 0 04335        LDQ I0
01212  0 02000 0 01215        TRA XS3
01213  0 50000 0 10514  XS2   CLA M8
01214  0 56000 0 10515        LDQ M9
01215  0 60100 0 10516  XS3   STO M10
01216 -0 60000 0 10517        STQ M11
01217 -0 63400 4 10346  XT    SXD T23,4
01220  0 50000 2 00000  XU    CLA 0,2
01221 -0 76000 0 00003  XU1   SSM                   OR TXI XU2
01222  0 40000 0 10330        ADD T11
01223  0 40000 0 04336        ADD I1
01224  0 73400 4 00000        PAX 0,4
01225  0 50000 4 00000        CLA 0,4
01226  0 60100 0 10354  XU2   STO T29
01227  0 56000 0 10513  XV    LDQ M7                  OR TXI XW,2,-10
01230  0 26000 2 00004        FMP 4,2
01231  0 07400 4 07027        TSX EXP,4
01232  0 00000 0 00144        HTR RCD                 NEGATIVE SYMM TEMP FACTOR
01233  0 60100 0 10355        STO T30
01234  0 56000 0 10355        LDQ T30
01235  0 26000 0 10354        FMP T29
01236  0 60100 0 10354        STO T29
01237  1 77773 2 01242        TXI XX,2,-5
01240  0 50000 0 04360  XW    CLA C1
01241  0 60100 0 10355        STO T30
01242  0 56000 0 10354  XX    LDQ T29
01243  0 26000 1 00000        FMP 0,1
01244  0 60100 0 10356        STO T31
01245  0 30000 0 10516        FAD M10
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      01246  0 60100 0 10516          STO M10
      01247  0 56000 0 10355  XY      LDQ T30                OR TXI XAB,1,-1
      01250  0 26000 1 00000          FMP 0,1
      01251  0 60100 1 00000          STO 0,1
      01252  1 77777 1 01253          TXI XY1,1,-1
      01253  0 56000 0 10354  XY1     LDQ T29
      01254  0 26000 0 04361          FMP C2
      01255  0 60100 0 10360          STO T33
      01256  0 76000 0 00002          CHS
      01257  0 60100 0 10361          STO T34
      01260  0 53400 4 04340          LXA I3,4
      01261  0 56000 0 10361  XY2     LDQ T34
      01262  0 26000 1 00000          FMP 0,1
      01263  0 60100 1 00000          STO 0,1
      01264  1 77777 1 01265          TXI XY3,1,-1
      01265  2 00001 4 01261  XY3     TIX XY2,4,1
      01266  0 56000 0 10356  XZ      LDQ T31                OR TXI XAA
      01267  0 26000 0 10513          FMP M7
      01270  0 76000 0 00002          CHS
      01271  0 60100 1 00000          STO 0,1
      01272  1 77777 1 01303          TXI XAB,1,-1
      01273  0 50200 0 10354  XAA     CLS T29
      01274  0 60100 0 10362          STO T35
      01275  0 53400 4 04343          LXA I6,4
      01276  0 56000 0 10362  XAA1    LDQ T35
      01277  0 26000 1 00000          FMP 0,1
      01300  0 60100 1 00000          STO 0,1
      01301  1 77777 1 01302          TXI XAA2,1,-1
      01302  2 00001 4 01276  XAA2    TIX XAA1,4,1
TD    01303  1 00000 0 01335  XAB     TXI XAF                OR LDQ T29
      01304  0 26000 1 00000          FMP 0,1
      01305  0 60100 0 10357          STO T32
      01306  0 30000 0 10517          FAD M11
      01307  0 60100 0 10517          STO M11
      01310  0 56000 0 10355  XAC     LDQ T30                OR TXI XAF,1,-1
      01311  0 26000 1 00000          FMP 0,1
      01312  0 60100 1 00000          STO 0,1
      01313  1 77777 1 01314          TXI XAC1,1,-1
      01314  0 53400 4 04340  XAC1    LXA I3,4
      01315  0 56000 0 10360  XAC2    LDQ T33
      01316  0 26000 1 00000          FMP 0,1
      01317  0 60100 1 00000          STO 0,1
      01320  1 77777 1 01321          TXI XAC3,1,-1
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01321  2 00001 4 01315  XAC3  TIX XAC2,4,1
01322  0 56000 0 10357  XAD   LDQ T32                 OR TXI XAE
01323  0 26000 0 10513        FMP M7
01324  0 76000 0 00002        CHS
01325  0 60100 1 00000        STO 0,1
01326  1 77777 1 01335        TXI XAF,1,-1
01327  0 53400 4 04343  XAE   LXA I6,4
01330  0 56000 0 10362  XAE1  LDQ T35
01331  0 26000 1 00000        FMP 0,1
01332  0 60100 1 00000        STO 0,1
01333  1 77777 1 01334        TXI XAE2,1,-1
01334  2 00001 4 01330  XAE2  TIX XAE1,4,1
01335 -0 53400 4 10346  XAF   LXD T23,4
01336  2 00001 4 01217        TIX XT,4,1
01337  0 56000 0 10513  XAG   LDQ M7
01340  0 26000 0 00000  XAG1  FMP 0                   ADDRESS TO BE SET
01341  0 07400 4 07027        TSX EXP,4
01342  0 00000 0 00144        HTR RCD                 NEGATIVE OVERALL TEMP FACTOR
01343  0 60100 0 10363        STO T36
01344  0 50000 0 10525        CLA T5
01345  0 40000 0 10512        ADD M6
01346  0 62100 0 01347        STA XAG2
01347  0 56000 0 00000  XAG2  LDQ 0                   ADDRESS TO BE SET
01350 -0 60000 0 10364        STQ T37
01351  0 26000 0 10363        FMP T36
01352  0 60100 0 10363        STO T36
TD 01353  1 00000 0 01354  XAH   TXI XAI               OR TXI XAK
01354  0 50000 0 10363  XAI   CLA T36                 OR TXI XAJ
01355  0 30000 0 10363        FAD T36
01356  0 60100 0 10365        STO T38
01357  0 56000 0 10365        LDQ T38
01360  0 26000 0 10516        FMP M10
01361  0 60100 0 10520        STO M12
TD 01362  1 00000 0 01463        TXI XAM
01363  0 56000 0 10516  XAJ   LDQ M10
01364  0 26000 0 10516        FMP M10
01365  0 60100 0 10367        STO T40
01366  0 56000 0 10517        LDQ M11
01367  0 26000 0 10517        FMP M11
01370  0 30000 0 10367        FAD T40
01371 -0 10000 0 01376        TNZ XAJ1
01372  0 60000 0 10520        STZ M12
01373  0 60000 0 10365        STZ T38
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      01374  0 60000 0 10366        STZ T39
TD    01375  1 00000 0 01463        TXI XAM
      01376  0 07400 4 06116  XAJ1  TSX SQRT,4
      01377  0 00000 0 00144        HTR RCD                NEGATIVE RADICAND
      01400  0 60100 0 10367        STO T40
      01401  0 56000 0 10367        LDQ T40
      01402  0 26000 0 10363        FMP T36
      01403  0 60100 0 10520        STO M12
      01404  0 50000 0 10363        CLA T36
      01405  0 24000 0 10367        FDH T40
      01406 -0 60000 0 10366        STQ T39
      01407  0 26000 0 10516        FMP M10
      01410  0 60100 0 10365        STO T38
      01411  0 56000 0 10366        LDQ T39
      01412  0 26000 0 10517        FMP M11
      01413  0 60100 0 10366        STO T39
TD    01414  1 00000 0 01463        TXI XAM
      01415  0 50000 0 10363  XAK   CLA T36                OR TXI XAL
      01416  0 30000 0 10363        FAD T36
      01417  0 60100 0 10365        STO T38
      01420  0 56000 0 10365        LDQ T38
      01421  0 26000 0 10365        FMP T38
      01422  0 60100 0 10365        STO T38
      01423  0 56000 0 10365        LDQ T38
      01424  0 26000 0 10516        FMP M10
      01425  0 60100 0 10365        STO T38
      01426  0 56000 0 10365        LDQ T38
      01427  0 26000 0 10516        FMP M10
      01430  0 60100 0 10520        STO M12
      01431  0 50000 0 10365        CLA T38
      01432  0 30000 0 10365        FAD T38
      01433  0 60100 0 10365        STO T38
TD    01434  1 00000 0 01473        TXI XAN
      01435  0 56000 0 10363  XAL   LDQ T36
      01436  0 26000 0 10363        FMP T36
      01437  0 60100 0 10365        STO T38
      01440  0 30000 0 10365        FAD T38
      01441  0 60100 0 10366        STO T39
      01442  0 56000 0 10516        LDQ M10
      01443  0 26000 0 10516        FMP M10
      01444  0 60100 0 10367        STO T40
      01445  0 56000 0 10517        LDQ M11
      01446  0 26000 0 10517        FMP M11
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     01447  0 30000 0 10367          FAD T40
     01450  0 60100 0 10367          STO T40
     01451  0 56000 0 10367          LDQ T40
     01452  0 26000 0 10365          FMP T38
     01453  0 60100 0 10520          STO M12
     01454  0 56000 0 10516          LDQ M10
     01455  0 26000 0 10366          FMP T39
     01456  0 60100 0 10365          STO T38
     01457  0 56000 0 10517          LDQ M11
     01460  0 26000 0 10366          FMP T39
     01461  0 60100 0 10366          STO T39
TD   01462  1 00000 0 01473          TXI XAN
     01463  0 50000 0 10520  XAM     CLA M12                OR TXI XAW
     01464  0 24000 0 10364          FDH T37
     01465 -0 60000 0 10523          STQ M15
     01466  0 56000 0 10513          LDQ M7
     01467  0 26000 0 10520          FMP M12
     01470  0 76000 0 00002          CHS
     01471  0 60100 0 10524          STO M16
TD   01472  1 00000 0 01507          TXI XAO
     01473  0 50000 0 10520  XAN     CLA M12                OR TXI XAW
     01474  0 24000 0 10364          FDH T37
     01475 -0 60000 0 10523          STQ M15
     01476  0 50000 0 10523          CLA M15
     01477  0 30000 0 10523          FAD M15
     01500  0 60100 0 10523          STO M15
     01501  0 56000 0 10513          LDQ M7
     01502  0 26000 0 10520          FMP M12
     01503  0 76000 0 00002          CHS
     01504  0 60100 0 10524          STO M16
     01505  0 30000 0 10524          FAD M16
     01506  0 60100 0 10524          STO M16
     01507  0 53400 4 10314  XAO     LXA T2,4
     01510  0 53400 2 10326          LXA T7,2
     01511  0 53400 1 10327          LXA T8,1
     01512 -0 63400 4 10346  XAP     SXD T23,4
     01513  0 53400 4 10370          LXA T41,4
     01514  0 56000 0 10365  XAQ     LDQ T38
     01515  0 26000 2 00000          FMP 0,2
     01516  0 60100 1 00000          STO 0,1
'D   01517  1 00000 0 01523  XAR     TXI XAS                OR LDQ T39
     01520  0 26000 2 00000  XAR1    FMP 0,2                ADDRESS TO BE SET
     01521  0 30000 1 00000          FAD 0,1
```

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     01522  0 60100 1 00000          STO 0,1
     01523  1 77777 2 01524  XAS     TXI XAS1,2,-1
     01524  1 77777 1 01525  XAS1    TXI XAT,1,-1
     01525  2 00001 4 01514  XAT     TIX XAQ,4,1
     01526 -0 53400 4 10346  XAU     LXD T23,4
     01527 -2 00001 4 01533          TNX XAW,4,1
TD   01530  1 00000 0 01512  XAV     TXI XAP                 OR NOP
     01531  2 00000 2 01512  XAV1    TIX XAP,2,0             DECREMENT TO BE SET
     01532  0 00000 0 00144          HTR RCD                 LOOKING FOR STORAGE THRU ZERO
     01533  0 50000 0 10510  XAW     CLA M4                  OR TXI XBK
     01534  0 56000 0 10520  XAW1    LDQ M12                 OR TXI XAW3
     01535  0 16200 0 01540          TQP XAW2
     01536 -0 76000 0 00003          SSM
TD   01537  1 00000 0 01541          TXI XAW3
     01540  0 76000 0 00003  XAW2    SSP
     01541  0 30200 0 10520  XAW3    FSB M12
     01542  0 60100 0 10521          STO M13
     01543  0 76000 0 00003          SSP
     01544  0 30000 0 10371          FAD T42
     01545  0 60100 0 10371          STO T42
     01546  0 56000 0 10511          LDQ M5
     01547  0 26000 0 10521          FMP M13
     01550  0 60100 0 10377          STO T48
     01551  0 56000 0 10377          LDQ T48
     01552  0 26000 0 10377          FMP T48
     01553  0 60100 0 10423          STO T57
     01554  0 30000 0 10373          FAD T44
     01555  0 60100 0 10373          STO T44
     01556  0 50000 0 10510          CLA M4
     01557  0 10000 0 01567          TZE XAW4
     01560  0 50000 0 10521          CLA M13
     01561  0 76000 0 00003          SSP
     01562  0 30000 0 10372          FAD T43
     01563  0 60100 0 10372          STO T43
     01564  0 50000 0 10423          CLA T57
     01565  0 30000 0 10374          FAD T45
     01566  0 60100 0 10374          STO T45
     01567  0 50000 0 10510  XAW4    CLA M4
     01570  0 76000 0 00003          SSP
     01571  0 30000 0 10375          FAD T46
     01572  0 60100 0 10375          STO T46
     01573  0 56000 0 10510          LDQ M4
     01574  0 26000 0 10511          FMP M5
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        01575   0 60100 0 10400          STO T49
        01576   0 56000 0 10400          LDQ T49
        01577   0 26000 0 10400          FMP T49
        01600   0 60100 0 10400          STO T49
        01601   0 30000 0 10376          FAD T47
        01602   0 60100 0 10376          STO T47
        01603   0 60000 0 10522  XAX     STZ M14                OR REJECTION TEST
        01604   0 02000 0 01705          TRA XAXX
                                 01605   BSS 64
        01705   0 50000 0 10522  XAXX    CLA M14
        01706  -0 10000 0 01717          TNZ XAY
        01707   0 50000 0 10511          CLA M5
        01710   0 10000 0 01717          TZE XAY
        01711   0 50000 0 10444          CLA T65
        01712   0 30000 0 04360          FAD C1
        01713   0 60100 0 10444          STO T65
        01714   0 50000 0 10445          CLA T66
        01715   0 30000 0 10423          FAD T57
        01716   0 60100 0 10445          STO T66
        01717   0 50000 0 10377  XAY     CLA T48                OR TXI XBH
        01720   0 76000 0 00003          SSP
        01721   0 30200 0 04366          FSB C7
        01722   0 12000 0 01732          TPL XBC
        01723   0 50000 0 10522  XAZ     CLA M14
        01724   0 10000 0 01727          TZE XBB
        01725   0 50000 0 04363  XBA     CLA C4
TD      01726   1 00000 0 01737          TXI XBF
        01727   0 50000 0 04362  XBB     CLA C3
        01730   0 60100 0 10401          STO T50
TD      01731   1 00000 0 01740  XBB1    TXI XBG                OR TXI XBH
        01732   0 50000 0 10522  XBC     CLA M14
        01733   0 10000 0 01736          TZE XBE
        01734   0 50000 0 04365  XBD     CLA C6
TD      01735   1 00000 0 01737          TXI XBF
        01736   0 50000 0 04364  XBE     CLA C5
        01737   0 60100 0 10401  XBF     STO T50
        01740   0 07400 4 05336  XBG     TSX SWTF,4             OR TRA XBG2,4, OR 6
        01741   0 00000 0 01753          PZE XBG1
        01742   0 07400 4 06147          TSX OUT,4
        01743   0 07400 4 05254          TSX ECHO,4
        01744   3 03734 0 04367          PTH C9,0,2012
        01745  -3 00004 0 10505          SVN M1,0,4
        01746  -3 00010 0 10506          SVN M2,0,8
```

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01747 -3 00014 0 10507          SVN M3,0,12
01750 -3 05721 0 10520          SVN M12,0,3025
01751 -3 05736 0 10516          SVN M10,0,3038
01752  1 00060 0 00003          PON U2,0,48
01753 -1 00000 0 00000  XBG1    FVE
01754  0 02000 0 02035          TRA XBH
01755  0 07400 4 05336  XBG2    TSX SWTF,4
01756  0 00000 0 01771          PZE XBG3
01757  0 07400 4 06147          TSX OUT,4
01760  0 07400 4 05254          TSX ECHO,4
01761  3 03734 0 04367          PTH C9,0,2012
01762 -3 00004 0 10505          SVN M1,0,4
01763 -3 00010 0 10506          SVN M2,0,8
01764 -3 00014 0 10507          SVN M3,0,12
01765 -3 05721 0 10520          SVN M12,0,3025
01766 -3 05736 0 10516          SVN M10,0,3038
01767 -3 05753 0 10517          SVN M11,0,3051
01770  1 00060 0 00003          PON U2,0,48
01771 -1 00000 0 00000  XBG3    FVE
01772  0 02000 0 02035          TRA XBH
01773  0 07400 4 05336  XBG4    TSX SWTF,4
01774  0 00000 0 02012          PZE XBG5
01775  0 07400 4 06147          TSX OUT,4
01776  0 07400 4 05254          TSX ECHO,4
01777  3 03734 0 04367          PTH C9,0,2012
02000 -3 00004 0 10505          SVN M1,0,4
02001 -3 00010 0 10506          SVN M2,0,8
02002 -3 00014 0 10507          SVN M3,0,12
02003 -3 05721 0 10510          SVN M4,0,3025
02004 -3 05736 0 10520          SVN M12,0,3038
02005 -3 05753 0 10516          SVN M10,0,3051
02006 -3 05770 0 10521          SVN M13,0,3064
02007 -3 04033 0 10377          SVN T48,0,2075
02010  3 02072 0 10401          PTH T50,0,1082
02011  1 00060 0 00003          PON U2,0,48
02012 -1 00000 0 00000  XBG5    FVE
02013  0 02000 0 02035          TRA XBH
02014  0 07400 4 05336  XBG6    TSX SWTF,4
02015  0 00000 0 02034          PZE XBG7
02016  0 07400 4 06147          TSX OUT,4
02017  0 07400 4 05254          TSX ECHO,4
02020  3 03734 0 04367          PTH C9,0,2012
02021 -3 00004 0 10505          SVN M1,0,4
```

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02022 -3 00010 0 10506          SVN M2,0,8
02023 -3 00014 0 10507          SVN M3,0,12
02024 -3 05721 0 10510          SVN M4,0,3025
02025 -3 05736 0 10520          SVN M12,0,3038
02026 -3 05753 0 10516          SVN M10,0,3051
02027 -3 05770 0 10517          SVN M11,0,3064
02030 -3 06005 0 10521          SVN M13,0,3077
02031 -3 04050 0 10377          SVN T48,0,2088
02032  3 02107 0 10401          PTH T50,0,1095
02033  1 00060 0 00003          PON U2,0,48
02034 -1 00000 0 00000  XBG7    FVE
02035  0 76600 0 00225  XBH     WTB U3                  OR TXI XA
02036  0 53400 1 04344          LXA I7,1
02037  0 70000 1 10514  XBH1    CPY M1+7,1
02040  2 00001 1 02037          TIX XBH1,1,1
02041  0 53400 1 10313          LXA T4,1
02042 -3 00000 1 02047          TXL XBH3,1,0
02043  0 53400 2 10330          LXA T11,2
02044  0 70000 2 00000  XBH2    CPY 0,2
02045 -2 00001 1 02047          TNX XBH3,1,1
02046  1 77777 2 02044          TXI XBH2,2,-1
02047  0 70000 0 10514  XBH3    CPY M8
02050  0 70000 0 10515          CPY M9
02051  0 70000 0 10516  XBH4    CPY M10                 OR TXI XA
02052  0 70000 0 10517          CPY M11
02053  0 70000 0 10520          CPY M12
02054  0 70000 0 10521  XBH5    CPY M13                 OR TXI XA
02055  0 70000 0 10522          CPY M14
02056  0 70000 0 10523          CPY M15
02057  0 70000 0 10524          CPY M16
02060  0 53400 1 10331          LXA T9,1
02061  0 53400 2 10327          LXA T8,2
02062  0 70000 2 00000  XBH6    CPY 0,2
02063 -2 00001 1 00725          TNX XA,1,1
02064  1 77777 2 02062          TXI XBH6,2,-1
02065  0 50000 0 10375  XBI     CLA T46                 OR TRA XSA
02066 -0 10000 0 02072          TNZ XBI1
02067  0 60000 0 10402          STZ T51
02070  0 60000 0 10403          STZ T52
TD 02071  1 00000 0 02100       TXI XBI2
02072  0 50000 0 10371  XBI1    CLA T42
02073  0 24000 0 10375          FDH T46
02074 -0 60000 0 10402          STQ T51
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        02075  0 50000 0 10372          CLA T43
        02076  0 24000 0 10375          FDH T46
        02077 -0 60000 0 10403          STQ T52
        02100  0 50000 0 10373  XBI2    CLA T44
        02101  0 07400 4 06116          TSX SQRT,4
        02102  0 00000 0 00144          HTR RCD                 NEGATIVE RADICAND
        02103  0 60100 0 10373          STO T44
        02104  0 50000 0 10374          CLA T45
        02105  0 07400 4 06116          TSX SQRT,4
        02106  0 00000 0 00144          HTR RCD                 NEGATIVE RADICAND
        02107  0 60100 0 10374          STO T45
        02110  0 50000 0 10376          CLA T47
        02111  0 07400 4 06116          TSX SQRT,4
        02112  0 00000 0 00144          HTR RCD                 NEGATIVE RADICAND
        02113  0 60100 0 10376          STO T47
        02114 -0 10000 0 02120          TNZ XBI3
        02115  0 60000 0 10404          STZ T53
        02116  0 60000 0 10405          STZ T54
TD      02117  1 00000 0 02126          TXI XBI4
        02120  0 50000 0 10373  XBI3    CLA T44
        02121  0 24000 0 10376          FDH T47
        02122 -0 60000 0 10404          STQ T53
        02123  0 50000 0 10374          CLA T45
        02124  0 24000 0 10376          FDH T47
        02125 -0 60000 0 10405          STQ T54
        02126  0 07400 4 06147  XBI4    TSX OUT,4
        02127  0 07400 4 05254          TSX ECHO,4
        02130  3 27451 0 10406          PTH T55,0,12073
        02131  3 02066 0 04362          PTH C3,0,1078
        02132  1 00001 0 00003          PON U2,0,1
        02133 -1 00000 0 00364          FVE 244
        02134  0 07400 4 06147          TSX OUT,4
        02135  0 07400 4 05254          TSX ECHO,4
        02136  3 17560 0 04766          PTH C83,0,8048
        02137  3 11727 0 04371          PTH C19,0,5079
        02140  1 00000 0 00003          PON U2,0,0
        02141 -1 00000 0 00364          FVE 244
        02142  0 07400 4 06147          TSX OUT,4
        02143  0 07400 4 05254          TSX ECHO,4
        02144  3 03734 0 04376          PTH C20,0,2012
        02145  3 05724 0 04403          PTH C22,0,3028
        02146 -3 05762 0 10371          SVN T42,0,3058
        02147 -3 05777 0 10375          SVN T46,0,3071
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02150 -3 06011 0 10402        SVN T51,0,3081
02151  1 00000 0 00003        PON U2,0,0
02152 -1 00000 0 00364        FVE 244
02153  0 07400 4 06147        TSX OUT,4
02154  0 07400 4 05254        TSX ECHO,4
02155  3 03734 0 04376        PTH C20,0,2012
02156  3 05724 0 04406        PTH C23,0,3028
02157 -3 05762 0 10372        SVN T43,0,3058
02160 -3 05777 0 10375        SVN T46,0,3071
02161 -3 06011 0 10403        SVN T52,0,3081
02162  1 00000 0 00003        PON U2,0,0
02163 -1 00000 0 00364        FVE 244
02164  0 07400 4 06147        TSX OUT,4
02165  0 07400 4 05254        TSX ECHO,4
02166  3 05712 0 04400        PTH C21,0,3018
02167  3 05735 0 04403        PTH C22,0,3037
02170 -3 05762 0 10373        SVN T44,0,3058
02171 -3 05777 0 10376        SVN T47,0,3071
02172 -3 06011 0 10404        SVN T53,0,3081
02173  1 00000 0 00003        PON U2,0,0
02174 -1 00000 0 00364        FVE 244
02175  0 07400 4 06147        TSX OUT,4
02176  0 07400 4 05254        TSX ECHO,4
02177  3 05712 0 04400        PTH C21,0,3018
02200  3 05735 0 04406        PTH C23,0,3037
02201 -3 05762 0 10374        SVN T45,0,3058
02202 -3 05777 0 10376        SVN T47,0,3071
02203 -3 06011 0 10405        SVN T54,0,3081
02204  1 00000 0 00003        PON U2,0,0
02205 -1 00000 0 00364        FVE 244
02206  0 50000 0 10444        CLA T65
02207  0 30200 0 10446        FSB T67
02210 -0 12000 0 02237        TMI XBI11
02211  0 10000 0 02237        TZE XBI11
02212  0 60100 0 10447        STO T68
02213  0 50000 0 10445        CLA T66
02214  0 24000 0 10447        FDH T68
02215 -0 60000 0 10447        STQ T68
02216  0 50000 0 10445        CLA T66
02217  0 07400 4 06116        TSX SQRT,4
02220  0 00000 0 00144        HTR RCD              NEGATIVE RADICAND
02221  0 60100 0 10503        STO T95
02222  0 50000 0 10447        CLA T68
```

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02223  0 07400 4 06116        TSX SQRT,4
02224  0 00000 0 00144        HTR RCD                 NEGATIVE RADICAND
02225  0 60100 0 10447        STO T68
02226  0 07400 4 06147        TSX OUT,4
02227  0 07400 4 05254        TSX ECHO,4
02230  3 31426 0 04650        PTH C63,0,13078
02231 -3 05762 0 10503        SVN T95,0,3058
02232 -3 00104 0 10444        SVN T65,0,68
02233 -3 00110 0 10446        SVN T67,0,72
02234 -3 06011 0 10447        SVN T68,0,3081
02235  1 00000 0 00003        PON U2,0,0
02236 -1 00000 0 00364        FVE 244
02237  0 07400 4 06147  XBI11 TSX OUT,4
02240  0 07400 4 05254        TSX ECHO,4
02241 -1 00000 0 00361        FVE 241
02242  0 02000 0 03162        TRA XSA
02243  0 50000 0 10516  XBK   CLA M10                 OR TXI XAY
02244  0 60100 0 10514        STO M8
02245  0 50000 0 10517        CLA M11
02246  0 60100 0 10515        STO M9
TD 02247  1 00000 0 01717        TXI XAY
02250  0 76200 0 00321  XDA   RCD
02251  0 07400 4 05363        TSX DBD1,4
02252  0 00000 0 06100        PZE BUFFER
02253  0 00000 0 00144        HTR RCD                 END OF FILE
02254  0 07400 4 05030        TSX IFF,4
02255  0 04356 0 06113        PZE BUFFER+11,0,IS
02256  0 02000 0 02250        TRA XDA
02257  0 53400 1 04350  XDB   LXA I12,1
02260  0 50000 0 04466        CLA C28
02261  0 60100 0 02265        STO XDC1
02262  0 50000 0 04467        CLA C29
02263  0 60100 0 02273        STO XDD1
02264  0 07400 4 05573  XDC   TSX FILE,4
02265  0 00000 0 00000  XDC1  PZE                     TO BE SET
02266  0 00000 0 00144        HTR RCD                 ERROR RETURN FROM FILE
02267  0 50000 0 10424        CLA T58
02270  0 40200 0 04362        SUB C3
02271  0 10000 0 02275        TZE XDE
02272  0 07400 4 05573  XDD   TSX FILE,4
02273  0 00000 0 00000  XDD1  PZE                     TO BE SET
02274  0 00000 0 00144        HTR RCD                 ERROR RETURN FROM FILE
02275 -2 00001 1 02303  XDE   TNX XDFF,1,1
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```
      02276  0 50000 0 02265  XDF    CLA XDC1
      02277  0 40000 0 04470         ADD C30
      02300  0 62200 0 02265         STD XDC1
      02301  0 62200 0 02273         STD XDD1
TD    02302  1 00000 0 02264         TXI XDC
      02303  0 07400 4 02305  XDFF   TSX XDG,4
      02304  0 02000 0 00471         TRA XCC
      02305 -0 63400 4 10422  XDG    SXD T56,4
      02306  0 53400 4 10305         LXA S1,4
      02307  3 00004 4 02317         TXH XDG1,4,4
      02310  0 50000 4 04314         CLA 1XEC1+1,4
      02311  0 60100 0 02722         STO XEC1
      02312  0 02000 4 02317         TRA XDG1,4
TD    02313  1 00000 0 02350         TXI XDG5
TD    02314  1 00000 0 02336         TXI XDG4
TD    02315  1 00000 0 02331         TXI XDG3
TD    02316  1 00000 0 02320         TXI XDG2
      02317  0 00000 0 00144  XDG1   HTR RCD                MODE NOT SPECIFIED
      02320  0 50000 0 04336  XDG2   CLA I1
      02321  0 60100 0 10311         STO S5
      02322  0 60100 0 10321         STO S12
      02323  0 60100 0 10323         STO S14
      02324  0 50000 0 04337         CLA I2
      02325  0 60100 0 10312         STO S6
      02326  0 60100 0 10322         STO S13
      02327  0 50000 0 04160         CLA 1XSB
      02330  0 02000 0 02361         TRA XDG6
      02331  0 50000 0 04337  XDG3   CLA I2
      02332  0 60100 0 10321         STO S12
      02333  0 60100 0 10322         STO S13
      02334  0 50000 0 04160         CLA 1XSB
      02335  0 02000 0 02361         TRA XDG6
      02336  0 50000 0 04336  XDG4   CLA I1
      02337  0 60100 0 10311         STO S5
      02340  0 60100 0 10312         STO S6
      02341  0 60100 0 10322         STO S13
      02342  0 50000 0 04337         CLA I2
      02343  0 60100 0 10321         STO S12
      02344  0 50000 0 04340         CLA I3
      02345  0 60100 0 10323         STO S14
      02346  0 50000 0 04157         CLA 2XSB
      02347  0 02000 0 02361         TRA XDG6
      02350  0 50000 0 04336  XDG5   CLA I1
```

```
02351  0 60100 0 10311          STO S5
02352  0 60100 0 10312          STO S6
02353  0 50000 0 04337          CLA I2
02354  0 60100 0 10321          STO S12
02355  0 60100 0 10322          STO S13
02356  0 50000 0 04340          CLA I3
02357  0 60100 0 10323          STO S14
02360  0 50000 0 04157          CLA 2XSB
02361  0 60100 0 03164  XDG6    STO XSB
02362  0 53400 4 10306  XDH     LXA S2,4
02363  3 00002 4 02365          TXH XDH1,4,2
02364  3 00000 4 02366          TXH XDH2,4,0
02365  0 00000 0 00144  XDH1    HTR RCD                 S2 NOT SPECIFIED
02366  0 50000 4 04163  XDH2    CLA 1XAH+1,4
02367  0 60100 0 01353          STO XAH
02370  0 50000 4 04165          CLA 1XAW1+1,4
02371  0 60100 0 01534          STO XAW1
02372  0 50000 4 04316          CLA 1XEC2+1,4
02373  0 60100 0 02727          STO XEC2
02374  0 53400 4 10307          LXA S3,4
02375  3 00003 4 02377          TXH XDH3,4,3
02376  3 00000 4 02400          TXH XDH4,4,0
02377  0 00000 0 00144  XDH3    HTR RCD                 S3 NOT SPECIFIED
02400  0 50000 4 04153  XDH4    CLA 1XGA+1,4
02401  0 60100 0 03116          STO XGA
02402  0 50000 4 04144          CLA 1S3+1,4
02403  0 60100 0 10307          STO S3
02404  0 50000 4 04321          CLA 1XEC3+1,4
02405  0 60100 0 02734          STO XEC3
02406  0 53400 4 10307          LXA S3,4
02407  0 50000 4 04167          CLA 1XFF2+1,4
02410  0 60100 0 03104          STO XFF2
02411  0 50000 4 04171          CLA 1XG+1,4
02412  0 60100 0 01041          STO XG
02413  0 50000 4 04173          CLA 1XJ+1,4
02414  0 60100 0 01114          STO XJ
02415  0 50000 4 04175          CLA 1XM+1,4
02416  0 60100 0 01150          STO XM
02417  0 50000 4 04177          CLA 1XP+1,4
02420  0 60100 0 01172          STO XP
02421  0 50000 4 04201          CLA 1XV+1,4
02422  0 60100 0 01227          STO XV
02423  0 50000 4 04203          CLA 1XZ+1,4
```

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02424  0 60100 0 01266          STO XZ
02425  0 50000 4 04205          CLA 1XAD+1,4
02426  0 60100 0 01322          STO XAD
02427  0 50000 4 04207          CLA 1T41+1,4
02430  0 60100 0 10370          STO T41
02431  0 62100 0 01520          STA XAR1
02432  0 76700 0 00022          ALS 18
02433  0 62200 0 01531          STD XAV1
02434  0 62200 0 04102          STD XWU
02435  0 50000 4 04150          CLA 1XWD+1,4
02436  0 60100 0 03747          STO XWD
02437  0 50000 4 04146          CLA 1XWP1+1,4
02440  0 60100 0 03773          STO XWP1
02441  0 53400 4 10310          LXA S4,4
02442  3 00003 4 02444          TXH XDH5,4,3
02443  3 00000 4 02445          TXH XDH6,4,0
02444  0 00000 0 00144  XDH5    HTR RCD                 S4 NOT SPECIFIED
02445  0 50000 4 04212  XDH6    CLA 1XCH+1,4
02446  0 60100 0 00666          STO XCH
02447  0 50000 4 04215          CLA 1XAY+1,4
02450  0 60100 0 01717          STO XAY
02451  0 50000 4 04220          CLA 1XBB1+1,4
02452  0 60100 0 01731          STO XBB1
02453  0 50000 4 04324          CLA 1XEC4+1,4
02454  0 60100 0 02741          STO XEC4
02455  0 53400 4 10311          LXA S5,4
02456  3 00002 4 02460          TXH XDH7,4,2
02457  3 00000 4 02461          TXH XDH8,4,0
02460  0 00000 0 00144  XDH7    HTR RCD                 S5 NOT SPECIFIED
02461  0 50000 4 04222  XDH8    CLA 1XBH+1,4
02462  0 60100 0 02035          STO XBH
02463  0 50000 4 04155          CLA 1XCF+1,4
02464  0 60100 0 00630          STO XCF
02465  0 50000 4 04157          CLA 1XSA+1,4
02466  0 60100 0 03162          STO XSA
02467  0 50000 4 04224          CLA 1XVI+1,4
02470  0 60100 0 04121          STO XVI
02471  0 53400 4 10312          LXA S6,4
02472  3 00002 4 02474          TXH XDH9,4,2
02473  3 00000 4 02475          TXH XDH10,4,0
02474  0 00000 0 00144  XDH9    HTR RCD                 S6 NOT SPECIFIED
02475  0 50000 4 04226  XDH10   CLA 1XAW+1,4
02476  0 60100 0 01533          STO XAW
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      02477  0 50000 4 04230          CLA 1XBI+1,4
      02500  0 60100 0 02065          STO XBI
      02501  0 50000 4 04331          CLA 1XEG1+1,4
      02502  0 60100 0 02763          STO XEG1
      02503  0 50000 0 10313          CLA S7
      02504  0 10000 0 02512          TZE XDH11
      02505  0 50000 0 04235          CLA 1XUO
      02506  0 60100 0 03631          STO XUO
      02507  0 50000 0 04231          CLA 1XFF1
      02510  0 56000 0 04233          LDQ 1XU1
TD    02511  1 00000 0 02516          TXI XDH12
      02512  0 50000 0 04234  XDH11   CLA 2XUO
      02513  0 60100 0 03631          STO XUO
      02514  0 50000 0 04230          CLA 2XFF1
      02515  0 56000 0 04232          LDQ 2XU1
      02516  0 60100 0 03076  XDH12   STO XFF1
      02517 -0 60000 0 01221          STQ XU1
      02520  0 53400 4 10315          LXA S9,4
      02521  3 00002 4 02523          TXH XDH13,4,2
      02522  3 00000 4 02524          TXH XDH14,4,0
      02523  0 00000 0 00144  XDH13   HTR RCD                 S9 NOT SPECIFIED
      02524  0 50000 4 04240  XDH14   CLA 1XN+1,4
      02525  0 60100 0 01157          STO XN
      02526  0 50000 4 04242          CLA 1XAB+1,4
      02527  0 60100 0 01303          STO XAB
      02530  0 50000 4 04244          CLA 1XAI+1,4
      02531  0 60100 0 01354          STO XAI
      02532  0 50000 4 04246          CLA 1XAK+1,4
      02533  0 60100 0 01415          STO XAK
      02534  0 50000 4 04250          CLA 1XAR+1,4
      02535  0 60100 0 01517          STO XAR
      02536  0 50000 4 04252          CLA 1XAV+1,4
      02537  0 60100 0 01530          STO XAV
      02540  0 50000 4 04333          CLA 1XEK1+1,4
      02541  0 60100 0 03010          STO XEK1
      02542  0 53400 4 10317          LXA S15,4
      02543  3 00002 4 02545          TXH XDH15,4,2
      02544  3 00000 4 02546          TXH XDH16,4,0
      02545  0 00000 0 00144  XDH15   HTR RCD                 S15 NOT SPECIFIED
      02546  0 50000 4 04137  XDH16   CLA 1XD+1,4
      02547  0 60100 0 00777          STO XD
      02550  0 50000 4 04141          CLA 1XF+1,4
      02551  0 60100 0 01001          STO XF
```

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02552   0 50000 4 04335          CLA 1XEK2+1,4
02553   0 60100 0 03021          STO XEK2
02554   0 53400 4 10321          LXA S12,4
02555   0 50000 4 04254          CLA 1XS1+1,4
02556   0 60100 0 01210          STO XS1
02557   0 50000 4 04256          CLA 1XBK+1,4
02560   0 60100 0 02243          STO XBK
02561   0 53400 4 10322          LXA S13,4
02562   0 50000 4 04260          CLA 1XL+1,4
02563   0 60100 0 01141          STO XL
02564   0 50000 4 04262          CLA 1XO+1,4
02565   0 60100 0 01163          STO XO
02566   0 50000 4 04264          CLA 1XY+1,4
02567   0 60100 0 01247          STO XY
02570   0 50000 4 04266          CLA 1XAC+1,4
02571   0 60100 0 01310          STO XAC
02572   0 50000 4 04270          CLA 1XAM+1,4
02573   0 60100 0 01463          STO XAM
02574   0 50000 4 04272          CLA 1XAN+1,4
02575   0 60100 0 01473          STO XAN
02576   0 53400 4 10323          LXA S14,4
02577   0 50000 4 04275          CLA 1XBH4+1,4
02600   0 60100 0 02051          STO XBH4
02601   0 50000 4 04300          CLA 1XBH5+1,4
02602   0 60100 0 02054          STO XBH5
02603   0 50000 4 04327          CLA 1XEE1+1,4
02604   0 60100 0 02750          STO XEE1
02605   0 50000 0 04337  XDI     CLA I2
02606   0 40200 0 10312          SUB S6
02607   0 76700 0 00001          ALS 1
02610   0 40000 0 10315          ADD S9
02611   0 73400 4 00000          PAX 0,4
02612   0 50000 4 04304          CLA 1XCH5+1,4
02613   0 60100 0 00714          STO XCH5
02614   0 50000 4 04310          CLA 1XBG+1,4
02615   0 60100 0 01740          STO XBG
02616   0 56000 0 10314  XDJ     LDQ S8
02617   0 20000 0 04342          MPY I5
02620   0 20000 0 10307          MPY S3
02621  -0 60000 0 10331          STQ T9
02622   0 53400 4 10322          LXA S13,4
02623  -3 00001 4 02625          TXL XDJ1,4,1
02624   0 56000 0 10314          LDQ S8
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```
02625  0 20000 0 10315  XDJ1  MPY S9
02626 -0 60000 0 10332         STQ T10
02627  0 50000 0 04337         CLA I2
02630  0 40200 0 10317         SUB S15
02631  0 60100 0 10443         STO T64
02632  0 56000 0 10443         LDQ T64
02633  0 20000 0 04343         MPY I6
02634  0 20000 0 10316         MPY S10
02635 -0 60000 0 10443         STQ T64
T 02636 -0 75400 0 00000       PXD
02637  0 76000 0 00006         COM
02640 -0 73400 1 00000         PDX 0,1
02641 -0 75400 1 00000         PXD 0,1
02642  0 77100 0 00022         ARS 18
02643  0 60100 0 10425         STO T59
02644  0 50000 0 10525         CLA T5
02645  0 40000 0 04336         ADD I1
02646  0 40000 0 10320         ADD S11
02647  0 62100 0 01340         STA XAG1
02650  0 62100 0 03505         STA XTW
02651  0 62100 0 03535         STA XTY1
02652  0 62100 0 03547         STA XUB1
02653  0 62100 0 03550         STA XUB2
02654  0 62100 0 03742         STA XWA
02655  0 62100 0 03765         STA XWN
02656  0 60100 0 10324         STO T61
02657  0 40000 0 10443         ADD T64
02660  0 60100 0 10325         STO T6
02661  0 40000 0 10331         ADD T9
02662  0 60100 0 10330         STO T11
02663  0 40000 0 10313         ADD S7
02664  0 60100 0 10326         STO T7
02665  0 40000 0 10332         ADD T10
02666  0 60100 0 10327         STO T8
02667  0 53400 4 10305         LXA S1,4
02670 -3 00002 4 02674         TXL XDJ2,4,2
02671  0 40000 0 05024         ADD C89
02672  0 40000 0 77760         ADD K1
02673  0 40000 0 10331         ADD T9
02674  0 34000 0 10425  XDJ2  CAS T59
02675  0 00000 0 00144         HTR RCD          PROBLEM EXCEEDS MEMORY CAPACITY
02676  0 76100 0 00000         NOP
02677  0 53400 4 04342         LXA I5,4
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      02700  0 50000 4 10331  XDJ3  CLA T61+5,4
      02701  0 76000 0 00006        COM
      02702  0 60100 4 10331        STO T61+5,4
      02703  2 00001 4 02700        TIX XDJ3,4,1
      02704  0 50000 0 10330        CLA T11
      02705  0 76700 0 00022        ALS 18
      02706  0 62200 0 03331        STD XTC1
      02707  0 62200 0 04124        STD XVI1
      02710 -0 53400 4 10422  XDK   LXD T56,4
      02711  0 02000 4 00001        TRA 1,4
      02712  0 07400 4 06147  XEB   TSX OUT,4
      02713  0 07400 4 05254        TSX ECHO,4
      02714  3 27451 0 10406        PTH T55,0,12073
      02715  3 02066 0 04362        PTH C3,0,1078
      02716 -1 00000 0 00364        FVE 244
      02717  0 07400 4 06147  XEC   TSX OUT,4
      02720  0 07400 4 05254        TSX ECHO,4
      02721  3 01756 0 04471        PTH C31,0,1006
      02722  0 00000 0 00000  XEC1  PZE                    TO BE SET
      02723 -1 00000 0 00364        FVE 244
      02724  0 07400 4 06147        TSX OUT,4
      02725  0 07400 4 05254        TSX ECHO,4
      02726  3 03734 0 04521        PTH C36,0,2012
      02727  0 00000 0 00000  XEC2  PZE                    TO BE SET
      02730 -1 00000 0 00000        FVE
      02731  0 07400 4 06147        TSX OUT,4
      02732  0 07400 4 05254        TSX ECHO,4
      02733  3 07670 0 04526        PTH C39,0,4024
      02734  0 00000 0 00000  XEC3  PZE                    TO BE SET
      02735 -1 00000 0 00000        FVE
      02736  0 07400 4 06147        TSX OUT,4
      02737  0 07400 4 05254        TSX ECHO,4
      02740  3 03734 0 04536        PTH C42,0,2012
      02741  0 00000 0 00000  XEC4  PZE                    TO BE SET
      02742 -1 00000 0 00000        FVE
      02743  0 53400 4 10311        LXA S5,4
      02744  3 00001 4 02753        TXH XEF,4,1
      02745  0 07400 4 06147  XEE   TSX OUT,4
      02746  0 07400 4 05254        TSX ECHO,4
      02747  3 05712 0 04544        PTH C46,0,3018
      02750  0 00000 0 00000  XEE1  PZE                    TO BE SET
      02751 -1 00000 0 00000        FVE
TD    02752  1 00000 0 02760        TXI XEG
```

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      02753  0 07400 4 06147  XEF    TSX OUT,4
      02754  0 07400 4 05254         TSX ECHO,4
      02755  3 05712 0 04544         PTH C46,0,3018
      02756  3 01775 0 04543         PTH C45,0,1021
      02757 -1 00000 0 00000         FVE
      02760  0 07400 4 06147  XEG    TSX OUT,4
      02761  0 07400 4 05254         TSX ECHO,4
      02762  3 11646 0 04563         PTH C50,0,5030
      02763  0 00000 0 00000  XEG1   PZE                    TO BE SET
      02764 -1 00000 0 00000         FVE
      02765  0 50000 0 10313  XEH    CLA S7
      02766 -0 10000 0 02774         TNZ XEJ
      02767  0 07400 4 06147  XEI    TSX OUT,4
      02770  0 07400 4 05254         TSX ECHO,4
      02771  3 03734 0 04574         PTH C53,0,2012
      02772 -1 00000 0 00000         FVE
TD    02773  1 00000 0 03001         TXI XEK
      02774  0 07400 4 06147  XEJ    TSX OUT,4
      02775  0 07400 4 05254         TSX ECHO,4
      02776  3 13624 0 04576         PTH C54,0,6036
      02777 -0 00016 0 10313         FOR S7,0,14
      03000 -1 00000 0 00000         FVE
      03001  0 07400 4 06147  XEK    TSX OUT,4
      03002  0 07400 4 05254         TSX ECHO,4
      03003  3 13624 0 04604         PTH C55,0,6036
      03004 -0 00047 0 10314         FOR S8,0,39
      03005 -1 00000 0 00000         FVE
      03006  0 07400 4 06147         TSX OUT,4
      03007  0 07400 4 05254         TSX ECHO,4
      03010  0 00000 0 00000  XEK1   PZE                    TO BE SET
      03011 -1 00000 0 00000         FVE
      03012  0 07400 4 06147         TSX OUT,4
      03013  0 07400 4 05254         TSX ECHO,4
      03014  3 17560 0 04617         PTH C58,0,8048
      03015 -0 00062 0 10316         FOR S10,0,50
      03016 -1 00000 0 00000         FVE
      03017  0 07400 4 06147         TSX OUT,4
      03020  0 07400 4 05254         TSX ECHO,4
      03021  0 00000 0 00000  XEK2   PZE                    TO BE SET
      03022 -1 00000 0 00000         FVE
      03023  0 07400 4 06147         TSX OUT,4
      03024  0 07400 4 05254         TSX ECHO,4
      03025  3 11646 0 04627         PTH C59,0,5030
```

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03026 -0 00034 0 10320          FOR S11,0,28
03027 -1 00000 0 00000          FVE
03030  0 07400 4 06147          TSX OUT,4
03031  0 07400 4 05254          TSX ECHO,4
03032 -1 00000 0 00361          FVE 241
03033  0 02000 0 00472  XEL     TRA XRA
03034  0 50000 0 10320  XFB     CLA T3
03035  0 40000 0 04336          ADD I1
03036  0 73400 1 00000          PAX 0,1
03037  0 50000 0 10525          CLA T5
03040  0 76000 0 00006          COM
03041  0 73400 2 00000          PAX 0,2
03042  0 76200 0 00321  XFC     RCD
03043  0 07400 4 05363          TSX DBD1,4
03044  0 00000 0 06100          PZE BUFFER
03045  0 00000 0 00144          HTR RCD                 END OF FILE
03046  0 07400 4 05030          TSX IFF,4
03047  0 04355 0 06113          PZE BUFFER+11,0,IP
03050  0 02000 0 03042          TRA XFC
03051  0 07400 4 05135          TSX BLNK,4
03052  0 00002 0 06102          PZE BUFFER+2,0,2
03053  0 02000 0 03116          TRA XGA
03054  0 07400 4 05573          TSX FILE,4
03055 -2 00155 2 00000          MTW 0,2,109
03056  0 00000 0 00144          HTR RCD                 ERROR RETURN FROM FILE
03057  1 77777 2 03060          TXI XFD,2,-1
03060  2 00001 1 03042  XFD     TIX XFC,1,1
03061  0 53400 1 10314  XFE     LXA T2,1
03062  0 53400 2 10325          LXA T6,2
03063  0 76200 0 00321  XFF     RCD
03064  0 07400 4 05363          TSX DBD1,4
03065  0 00000 0 06100          PZE BUFFER
03066  0 00000 0 00144          HTR RCD                 END OF FILE
03067  0 07400 4 05030          TSX IFF,4
03070  0 04355 0 06113          PZE BUFFER+11,0,IP
03071  0 02000 0 03063          TRA XFF
03072  0 07400 4 05135          TSX BLNK,4
03073  0 00013 0 06113          PZE BUFFER+11,0,11
03074  0 02000 0 03116          TRA XGA
03075  0 07400 4 05573          TSX FILE,4
03076 -1 00153 2 00000  XFF1    MON 0,2,107             OR MTW 0,2,107
03077 -2 01456 2 00001          MTW 1,2,814
03100 -2 02761 2 00002          MTW 2,2,1521
```

```
03101 -2 04264 2 00003          MTW 3,2,2228
03102 -2 05567 2 00004          MTW 4,2,2935
03103  0 00000 0 00144          HTR RCD                 ERROR RETURN FROM FILE
03104  1 77773 2 03115  XFF2    TXI XFG,2,-5            OR TXI XFF3,2,-5
03105  0 07400 4 05573  XFF3    TSX FILE,4
03106 -2 07072 2 00000          MTW 0,2,3642
03107 -2 10375 2 00001          MTW 1,2,4349
03110 -2 11700 2 00002          MTW 2,2,5056
03111 -2 13203 2 00003          MTW 3,2,5763
03112 -2 14506 2 00004          MTW 4,2,6470
03113  0 00000 0 00144          HTR RCD                 ERROR RETURN FROM FILE
03114  1 77773 2 03115          TXI XFG,2,-5
03115  2 00001 1 03063  XFG     TIX XFF,1,1
03116  0 02000 0 00621  XGA     TRA XCE                 OR CLA I2
03117  0 60100 0 10307          STO S3
03120  0 07400 4 02305  XGB     TSX XDG,4
03121  0 56000 0 04342  XGC     LDQ I5
03122  0 20000 0 10314          MPY S8
03123 -0 60000 0 10476          STQ T90
03124  0 50000 0 10325          CLA T6
03125  0 40200 0 10476          SUB T90
03126  0 40000 0 04336          ADD I1
03127  0 73400 1 00000          PAX 0,1
03130  0 40200 0 10476          SUB T90
03131  0 40000 0 04342          ADD I5
03132  0 73400 2 00000          PAX 0,2
03133  0 53400 4 10314  XGD     LXA S8,4
03134  0 50000 1 00000  XGE     CLA 0,1
03135  0 60100 0 10477          STO T91
03136 -0 63400 1 10346          SXD T23,1
03137  0 53400 1 04343  XGF     LXA I6,1
03140  0 56000 0 10477  XGG     LDQ T91
03141  0 26000 1 10476          FMP T84+6,1
03142  0 60100 2 00000          STO 0,2
03143 -2 00001 1 03145  XGH     TNX XGJ,1,1
03144  1 77777 2 03140  XGI     TXI XGG,2,-1
03145 -2 00001 4 00621  XGJ     TNX XCE,4,1
03146  1 00017 2 03147  XGK     TXI XGL,2,15
03147 -0 53400 1 10346  XGL     LXD T23,1
03150  1 00005 1 03151          TXI XGM,1,5
03151  0 50000 1 00001  XGM     CLA 1,1
03152  0 60100 2 00006          STO 6,2
03153  0 50000 1 00002          CLA 2,1
```

```
03154  0 60100 2 00007          STO 7,2
03155  0 50000 1 00003          CLA 3,1
03156  0 60100 2 00010          STO 8,2
03157  0 50000 1 00004          CLA 4,1
03160  0 60100 2 00011          STO 9,2
03161  0 02000 0 03134          TRA XGE
03162  0 77000 0 00205  XSA     WEF U3                  OR TRA XSB
03163  0 77000 0 00205          WEF U3
03164  0 76200 0 00321  XSB     RCD                     OR TRA XVH
03165  0 07400 4 05363          TSX DBD1,4
03166  0 00000 0 06100          PZE BUFFER
03167  0 00000 0 03164          HTR XSB                 END OF FILE
03170  0 07400 4 05030  XSC     TSX IFF,4
03171  0 04353 0 06113          PZE BUFFER+11,0,IK
03172  0 02000 0 03164          TRA XSB
03173  0 07400 4 05135  XSD     TSX BLNK,4
03174  0 00002 0 06102          PZE BUFFER+2,0,2
03175  0 02000 0 03217          TRA XSK
03176  0 07400 4 05573  XSE     TSX FILE,4
03177 -1 00152 0 77761          MON K2,0,106
03200 -1 01310 0 77760          MON K1,0,712
03201 -2 00152 0 10446          MTW T67,0,106
03202  0 00000 0 00144          HTR RCD                 ERROR RETURN FROM FILE
03203  0 50000 0 77760          CLA K1
03204  0 76700 0 00001          ALS 1
03205  0 60100 0 77760          STO K1
03206  0 53400 1 77760  XSF     LXA K1,1
03207  0 76200 0 00321  XSG     RCD
03210  0 53400 2 04346          LXA I9,2
03211  0 70000 1 77760  XSH     CPY K1,1
03212  0 02000 0 03214          TRA XSH1
03213  0 00000 0 03207          HTR XSG                 END OF FILE
03214  0 70000 1 77761  XSH1    CPY K1+1,1
03215  2 00001 2 03211  XSI     TIX XSH,2,1
03216  2 00002 1 03207  XSJ     TIX XSG,1,2
03217  0 53400 1 77761  XSK     LXA K2,1
03220  3 00000 1 03223          TXH XSM,1,0
03221  0 60000 0 77760  XSL     STZ K1
03222  0 02000 0 03361          TRA XTO
03223  0 50000 0 10313  XSM     CLA S7
03224  0 60100 0 77763          STO K4
03225  0 50000 0 10305          CLA S1
03226  0 60100 0 77774          STO K13
```

```
03227  0 50000 0 77761  XSN   CLA K2
03230  0 40000 0 04336        ADD I1
03231  0 76500 0 00043        LRS 35
03232  0 20000 0 77761        MPY K2
03233  0 76500 0 00001        LRS 1
03234 -0 60000 0 77775        STQ K14
03235  0 50000 0 04665        CLA C64
03236  0 40200 0 77760        SUB K1
03237  0 60100 0 77776        STO K15
03240  0 40200 0 77761        SUB K2
03241  0 60100 0 77773        STO K12
03242  0 40200 0 77775        SUB K14
03243  0 60100 0 77775        STO K14
03244  0 40200 0 77761        SUB K2
03245  0 40200 0 04336        SUB I1
03246  0 76000 0 00006        COM
03247  0 60100 0 77771        STO K10
03250  0 50000 0 77775        CLA K14
03251  0 40200 0 04336        SUB I1
03252  0 76000 0 00006        COM
03253  0 62100 0 77777        STA K16
03254  0 50000 0 77773        CLA K12
03255  0 40200 0 04336        SUB I1
03256  0 76000 0 00006        COM
03257  0 76700 0 00022        ALS 18
03260  0 62200 0 77777        STD K16
03261  0 50000 0 77775        CLA K14
03262  0 40000 0 77761        ADD K2
03263  0 60100 0 77772        STO K11
03264  0 53400 4 77771  XSO   LXA K10,4
03265  0 60000 0 77762        STZ K3
03266  0 53400 2 10320  XSP   LXA S11,2
03267  0 53400 1 77760  XSQ   LXA K1,1
03270 -0 50000 1 77760  XSR   CAL K1,1
03271 -0 63400 1 77766        SXD K7,1
03272  0 53400 1 04351        LXA I36,1
03273 -0 76000 0 00001  XSS   PBT
03274  0 02000 0 03303        TRA XSU
03275  0 60200 0 77767  XST   SLW K8
03276  0 50000 0 77762        CLA K3
03277  0 40000 0 04336        ADD I1
03300  0 60100 0 77762        STO K3
03301 -0 50000 0 77767        CAL K8
```

```
03302  1 77777 4 03303          TXI XSU,4,-1
03303  0 76700 0 00001  XSU     ALS 1
03304 -2 00001 1 03307  XSV     TNX XSX,1,1
03305  2 00001 2 03273  XSW     TIX XSS,2,1
03306  0 02000 0 03315          TRA XTA
03307 -0 53400 1 77766  XSX     LXD K7,1
03310 -2 00001 1 03322          TNX XTB,1,1
03311  2 00001 2 03270  XSY     TIX XSR,2,1
03312 -0 50000 1 77760  XSZ     CAL K1,1
03313 -0 63400 1 77766          SXD K7,1
03314  0 53400 1 04351          LXA I36,1
03315  0 60200 0 77767  XTA     SLW K8
03316 -0 63400 1 77765          SXD K6,1
03317 -0 63400 4 77764          SXD K5,4
03320  0 50000 0 04336          CLA I1
03321  0 02000 0 03323          TRA XTB1
03322  0 50000 0 04337  XTB     CLA I2
03323  0 60100 0 77770  XTB1    STO K9
03324  0 76400 0 00205  XTC     BST U3
03325  0 76400 0 00205          BST U3
03326  0 76200 0 00225          RTB U3
03327  0 07400 4 00146          TSX WTB,4
03330  0 00000 0 00005          PZE U3
03331  0 00000 0 77323  XTC1    PZE -START,0,0        DECREMENT TO BE SET
03332  0 77200 0 00205          REW U3
03333  0 02000 0 00144          TRA RCD               ENTER OR-XLS3
03334  0 53400 1 04342  XTD     LXA I5,1              RETURN FROM OR XLS5
03335  0 76200 0 00225  XTD1    RTB U3
03336  2 00001 1 03335          TIX XTD1,1,1
03337  0 53400 4 04340  XTE     LXA I3,4
03340  0 76200 0 00225  XTF     RTB U3
03341 -0 76000 0 00012          RTT
03342  0 76100 0 00000          NOP
03343  0 53400 1 10326  XTG     LXA T7,1
03344  0 70000 0 10502          CPY T94
03345  0 70000 1 00000  XTH     CPY 0,1
03346  1 77777 1 03345  XTI     TXI XTH,1,-1
03347  0 00000 0 00144          HTR RCD               END OF FILE
03350  0 76600 0 00333  XTJ     IOD
03351 -0 76000 0 00012          RTT
03352  0 02000 0 03356          TRA XTL
03353  0 77200 0 00205  XTK     REW U3
03354  0 77200 0 00204          REW U1
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03355  0 02000 0 03361        TRA XTO
03356  0 76400 0 00205  XTL   BST U3
03357  2 00001 4 03340  XTM   TIX XTF,4,1
03360  0 00000 0 03337  XTN   HTR XTE                RTT FAILS 3 TIMES. START TO TRY AGAIN
03361  0 07400 4 06147  XTO   TSX OUT,4
03362  0 07400 4 05254        TSX ECHO,4
03363  3 27451 0 10406        PTH T55,0,12073
03364  3 02066 0 04362        PTH C3,0,1078
03365  1 00001 0 00003        PON U2,0,1
03366 -1 00000 0 00364        FVE 244
03367  0 50000 0 10445  XTOO  CLA T66
03370  0 30200 0 10502        FSB T94
03371  0 60100 0 10445        STO T66
03372  0 50000 0 10444        CLA T65
03373  0 30200 0 10446        FSB T67
03374  0 60100 0 10447        STO T68
03375  0 10000 0 03401        TZE XTOO1
03376  0 50000 0 10445        CLA T66
03377  0 24000 0 10447        FDH T68
03400 -0 60000 0 10447        STQ T68
03401  0 50000 0 10445  XTOO1 CLA T66
03402  0 07400 4 06116        TSX SQRT,4
03403 -0 76000 0 00003        SSM
03404  0 60100 0 10503        STO T95
03405  0 50000 0 10447        CLA T68
03406  0 07400 4 06116        TSX SQRT,4
03407 -0 76000 0 00003        SSM
03410  0 60100 0 10447        STO T68
03411  0 07400 4 06147  XTOO2 TSX OUT,4
03412  0 07400 4 05254        TSX ECHO,4
03413  3 03734 0 04776        PTH C84,0,2012
03414  3 11727 0 04371        PTH C19,0,5079
03415  1 00000 0 00003        PON U2,0,0
03416 -1 00000 0 00364        FVE 244
03417  0 07400 4 06147  XTOO3 TSX OUT,4
03420  0 07400 4 05254        TSX ECHO,4
03421  3 31426 0 04650        PTH C63,0,13078
03422 -3 05762 0 10503        SVN T95,0,3058
03423 -3 00104 0 10444        SVN T65,0,68
03424 -3 00110 0 10446        SVN T67,0,72
03425 -3 06011 0 10447        SVN T68,0,3081
03426  1 00000 0 00003        PON U2,0,0
03427 -1 00000 0 00364        FVE 244
```

```
03430  0 07400 4 06147  XT004 TSX OUT,4
03431  0 07400 4 05254        TSX ECHO,4
03432  3 11646 0 05000        PTH C85,0,5030
03433  1 00000 0 00003        PON U2,0,0
03434 -1 00000 0 00364        FVE 244
03435  0 50000 0 05334  XTPP  CLA SWTP7
03436  0 60100 0 05335        STO SWTP8
03437  0 76000 0 00164  XTPP1 SWT 4
03440  0 02000 0 03442        TRA XTPP2
03441  0 02000 0 03450        TRA XTPP3
03442  0 07400 4 06147  XTPP2 TSX OUT,4
03443  0 07400 4 05254        TSX ECHO,4
03444  3 23514 0 05005        PTH C86,0,10060
03445  3 04024 0 05017        PTH C87,0,2068
03446 -0 00027 0 04341        FOR I4,0,23
03447 -1 00000 0 00364        FVE 244
03450  0 07400 4 05311  XTPP3 TSX SWTP,4
03451  0 00000 0 03456        PZE XTPP4
03452  0 07400 4 06147        TSX OUT,4
03453  0 07400 4 05254        TSX ECHO,4
03454  3 23514 0 04666        PTH C65,0,10060
03455  1 00000 0 00003        PON U2,0,0
03456 -1 00000 0 00364  XTPP4 FVE 244
03457  0 50000 0 04700  XTP   CLA C66
03460  0 60100 0 10451        STO T70
03461  0 50000 0 04701        CLA C66+1
03462  0 60100 0 10452        STO T70+1
03463  0 50000 0 04336        CLA I1
03464  0 60100 0 10453        STO T71
03465  0 53400 2 10326  XTQ   LXA T7,2
03466  0 53400 1 10320        LXA S11,1
03467  0 53400 4 77760        LXA K1,4
03470  3 00000 4 03473        TXH XTS,4,0
03471  0 60000 0 77767  XTR   STZ K8
03472  0 02000 0 03475        TRA XTT
03473 -0 50000 4 77760  XTS   CAL K1,4
03474  0 60200 0 77767        SLW K8
03475 -0 63400 4 77766  XTT   SXD K7,4
03476  0 53400 4 04351        LXA I36,4
03477 -0 63400 4 77765  XTU   SXD K6,4
03500 -0 50000 0 77767        CAL K8
03501 -0 76000 0 00001        PBT
03502  0 02000 0 03537        TRA XUA
```

```
03503  0 76700 0 00001  XTV    ALS 1
03504  0 60200 0 77767         SLW K8
03505  0 50000 1 00000  XTW    CLA 0,1                ADDRESS TO BE SET
03506  0 60100 0 10454         STO T72
03507  0 30000 2 00000         FAD 0,2
03510  0 60100 0 10455         STO T73
03511  0 50000 2 00001         CLA 1,2
03512  0 07400 4 06116         TSX SQRT,4
03513  0 00000 0 00144         HTR RCD                INVERSE DIAGONAL IS NEGATIVE
03514  0 60100 0 10456         STO T74
03515  0 56000 0 10456         LDQ T74
03516  0 26000 0 10447         FMP T68
03517  0 60100 0 10456         STO T74
03520  0 07400 4 05311  XTX    TSX SWTP,4
03521  0 00000 0 03533         PZE XTX1
03522  0 07400 4 06147         TSX OUT,4
03523  0 07400 4 05254         TSX ECHO,4
03524  3 03735 0 10451         PTH T70,0,2013
03525 -0 00020 0 10453         FOR T71,0,16
03526 -3 07671 0 10454         SVN T72,0,4025
03527 -3 07704 2 00000         SVN 0,2,4036
03530 -3 07717 0 10455         SVN T73,0,4047
03531 -3 07732 0 10456         SVN T74,0,4058
03532  1 00000 0 00003         PON U2,0,0
03533 -1 00000 0 00364  XTX1   FVE 244
03534  0 50000 0 10455  XTY    CLA T73
03535  0 60100 1 00000  XTY1   STO 0,1                ADDRESS TO BE SET
03536  1 77776 2 03553  XTZ    TXI XUC,2,-2
03537  0 76700 0 00001  XUA    ALS 1
03540  0 60200 0 77767         SLW K8
03541  0 07400 4 05311  XUB    TSX SWTP,4
03542  0 00000 0 03552         PZE XUB3
03543  0 07400 4 06147         TSX OUT,4
03544  0 07400 4 05254         TSX ECHO,4
03545  3 03735 0 10451         PTH T70,0,2013
03546 -0 00020 0 10453         FOR T71,0,16
03547 -3 07671 1 00000  XUB1   SVN 0,1,4025           ADDRESS TO BE SET
03550 -3 07717 1 00000  XUB2   SVN 0,1,4047           ADDRESS TO BE SET
03551  1 00000 0 00003         PON U2,0,0
03552 -1 00000 0 00364  XUB3   FVE 244
03553 -2 00001 1 03564  XUC    TNX XUH,1,1
03554  0 50000 0 10453  XUD    CLA T71
03555  0 40000 0 04336         ADD I1
```

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03556  0 60100 0 10453          STO T71
03557 -0 53400 4 77765  XUE     LXD K6,4
03560  2 00001 4 03477          TIX XTU,4,1
03561 -0 53400 4 77766  XUF     LXD K7,4
03562  2 00001 4 03473          TIX XTS,4,1
03563  0 02000 0 03471          TRA XTR
03564 -3 00000 1 03574  XUH     TXL XUJ,1,0
03565  0 53400 1 04335  XUI     LXA I0,1
03566  0 60000 0 10453          STZ T71
03567  0 50000 0 04702          CLA C67
03570  0 60100 0 10451          STO T70
03571  0 50000 0 04703          CLA C67+1
03572  0 60100 0 10452          STO T70+1
03573  0 02000 0 03557          TRA XUE
03574  0 53400 4 10314  XUJ     LXA S8,4
03575  0 50000 0 04336  XUK     CLA I1
03576  0 60100 0 10453          STO T71
03577  0 53400 1 10325  XUL     LXA T6,1
03600 -0 63400 1 10457          SXD T75,1
03601 -0 63400 4 10460  XUM     SXD T76,4
03602  0 07400 4 05311  XUM1    TSX SWTP,4
03603  0 00000 0 03611          PZE XUM2
03604  0 07400 4 06147          TSX OUT,4
03605  0 07400 4 05254          TSX ECHO,4
03606  3 01756 0 04704          PTH C68,0,1006
03607 -0 00010 0 10453          FOR T71,0,8
03610  1 00000 0 00003          PON U2,0,0
03611 -1 00000 0 00364  XUM2    FVE 244
03612  0 50000 0 10370  XUN     CLA T41
03613  0 76700 0 00001          ALS 1
03614  0 73400 1 00000          PAX 0,1
03615  0 40000 0 04740          ADD C78
03616  0 62100 0 03652          STA XUV1
03617  0 40000 0 04336          ADD I1
03620  0 62100 0 03654          STA XUV2
03621 -3 00012 1 03625          TXL XUN1,1,10
03622  0 50000 0 04733          CLA C72
03623  0 56000 0 04734          LDQ C72+1
03624  0 02000 0 03627          TRA XUN2
03625  0 50000 0 04731  XUN1    CLA C71
03626  0 56000 0 04732          LDQ C71+1
03627  0 60100 0 04715  XUN2    STO C70
03630 -0 60000 0 04716          STQ C70+1
```

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03631 -0 50000 0 04735  XUO    CAL C75                OR TRA XUP
03632  0 02000 0 03634         TRA XUP1
03633 -0 50000 0 04736  XUP    CAL C76
03634  0 60200 0 03724  XUP1   SLW XVD1
03635  0 40000 0 04737         ADD C77
03636  0 60200 0 03725         SLW XVD2
03637 -0 53400 4 77765  XUQ    LXD K6,4
03640  2 00001 4 03651         TIX XUV,4,1
03641 -0 53400 4 77766  XUR    LXD K7,4
03642  2 00001 4 03645         TIX XUT,4,1
03643  0 60000 0 77767  XUS    STZ K8
03644  0 02000 0 03647         TRA XUU
03645 -0 50000 4 77760  XUT    CAL K1,4
03646  0 60200 0 77767         SLW K8
03647 -0 63400 4 77766  XUU    SXD K7,4
03650  0 53400 4 04351         LXA I36,4
03651 -0 63400 4 77765  XUV    SXD K6,4
03652  0 50000 1 00000  XUV1   CLA 0,1                ADDRESS TO BE SET
03653  0 60100 0 10451         STO T70
03654  0 50000 1 00000  XUV2   CLA 0,1                ADDRESS TO BE SET
03655  0 60100 0 10452         STO T70+1
03656 -0 63400 1 10461         SXD T77,1
03657 -0 53400 1 10457         LXD T75,1
03660 -0 50000 0 77767  XUW    CAL K8
03661 -0 76000 0 00001         PBT
03662  0 02000 0 03715         TRA XVC
03663  0 76700 0 00001  XUX    ALS 1
03664  0 60200 0 77767         SLW K8
03665  0 50000 1 00000  XUY    CLA 0,1
03666  0 30000 2 00000         FAD 0,2
03667  0 60100 0 10455         STO T73
03670  0 50000 2 00001         CLA 1,2
03671  0 07400 4 06116         TSX SQRT,4
03672  0 00000 0 00144         HTR RCD                INVERSE DIAGONAL IS NEGATIVE
03673  0 60100 0 10456         STO T74
03674  0 56000 0 10456         LDQ T74
03675  0 26000 0 10447         FMP T68
03676  0 60100 0 10456         STO T74
03677  0 07400 4 05311  XUZ    TSX SWTP,4
03700  0 00000 0 03711         PZE XUZ1
03701  0 07400 4 06147         TSX OUT,4
03702  0 07400 4 05254         TSX ECHO,4
03703  3 03734 0 10451         PTH T70,0,2012
```

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03704 -3 15561 1 00000          SVN 0,1,7025
03705 -3 15574 2 00000          SVN 0,2,7036
03706 -3 15607 0 10455          SVN T73,0,7047
03707 -3 15622 0 10456          SVN T74,0,7058
03710  1 00000 0 00003          PON U2,0,0
03711 -1 00000 0 00364  XUZ1    FVE 244
03712  0 50000 0 10455  XVA     CLA T73
03713  0 60100 1 00000          STO 0,1
03714  1 77776 2 03730  XVB     TXI XVE,2,-2
03715  0 76700 0 00001  XVC     ALS 1
03716  0 60200 0 77767          SLW K8
03717  0 07400 4 05311  XVD     TSX SWTP,4
03720  0 00000 0 03727          PZE XVD3
03721  0 07400 4 06147          TSX OUT,4
03722  0 07400 4 05254          TSX ECHO,4
03723  3 03734 0 10451          PTH T70,0,2012
03724 -3 15561 1 00000  XVD1    SVN 0,1,7025          OR FOR 0,1,21
03725 -3 15607 1 00000  XVD2    SVN 0,1,7047          OR FOR 0,1,43
03726  1 00000 0 00003          PON U2,0,0
03727 -1 00000 0 00364  XVD3    FVE 244
03730  1 77777 1 03731  XVE     TXI XVE1,1,-1
03731 -0 63400 1 10457  XVE1    SXD T75,1
03732 -0 53400 1 10461          LXD T77,1
03733  2 00002 1 03633          TIX XUP,1,2
03734 -0 53400 4 10460  XVF     LXD T76,4
03735 -2 00001 4 03742          TNX XWA,4,1
03736  0 50000 0 10453  XVG     CLA T71
03737  0 40000 0 04336          ADD I1
03740  0 60100 0 10453          STO T71
03741  0 02000 0 03601          TRA XUM
03742  0 50000 0 00000  XWA     CLA 0                 ADDRESS TO BE SET
03743  0 10000 0 03766          TZE XWO
03744  0 60100 0 10477  XWB     STO T91
03745  0 53400 1 10314  XWC     LXA S8,1
03746  0 53400 2 10325          LXA T6,2
03747  0 50000 0 10477  XWD     CLA T91               OR TRA XWH
03750  0 30000 2 00004          FAD 4,2
03751  0 60100 2 00004          STO 4,2
03752 -2 00001 1 03765  XWE     TNX XWN,1,1
03753  1 77773 2 03747  XWF     TXI XWD,2,-5
03754  1 77774 2 03755  XWH     TXI XWI,2,-4
03755  0 53400 4 04343  XWI     LXA I6,4
03756  0 56000 0 10477  XWJ     LDQ T91
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03757  0 26000 4 10476        FMP T84+6,4
03760  0 30000 2 00000        FAD 0,2
03761  0 60100 2 00000        STO 0,2
03762  1 77777 2 03763  XWK   TXI XWL,2,-1
03763  2 00001 4 03756  XWL   TIX XWJ,4,1
03764  2 00001 1 03754  XWM   TIX XWH,1,1
03765  0 60000 0 00000  XWN   STZ 0                    ADDRESS TO BE SET
03766  0 53400 1 10314  XWO   LXA S8,1
03767  0 53400 2 10325        LXA T6,2
03770  0 50000 0 04336        CLA I1
03771  0 60100 0 10453        STO T71
03772  0 76100 0 00000  XWP   NOP                      TRANSFER TO RESET RELATIONS BETWEEN X,Y,Z
03773  0 50000 2 00004  XWP1  CLA 4,2                  OR TRA XWQ
03774 -0 12000 0 04071        TMI XWS
03775  0 02000 0 04101        TRA XWT
03776  0 76100 0 00000  XWQ   NOP                      TRANSFER TO RESET RELATIONS BETWEEN BETAS
03777  0 50000 2 00004  XWR   CLA 4,2
04000 -0 12000 0 04071        TMI XWS
04001  0 50000 2 00005        CLA 5,2
04002 -0 12000 0 04071        TMI XWS
04003  0 50000 2 00006        CLA 6,2
04004 -0 12000 0 04071        TMI XWS
04005  0 56000 2 00011        LDQ 9,2
04006  0 26000 2 00011        FMP 9,2
04007  0 60100 0 10501        STO T93
04010  0 56000 2 00005        LDQ 5,2
04011  0 26000 2 00006        FMP 6,2
04012  0 30200 0 10501        FSB T93
04013 -0 12000 0 04071        TMI XWS
04014  0 56000 2 00010        LDQ 8,2
04015  0 26000 2 00010        FMP 8,2
04016  0 60100 0 10501        STO T93
04017  0 56000 2 00004        LDQ 4,2
04020  0 26000 2 00006        FMP 6,2
04021  0 30200 0 10501        FSB T93
04022 -0 12000 0 04071        TMI XWS
04023  0 56000 2 00007        LDQ 7,2
04024  0 26000 2 00007        FMP 7,2
04025  0 60100 0 10501        STO T93
04026  0 56000 2 00004        LDQ 4,2
04027  0 26000 2 00005        FMP 5,2
04030  0 30200 0 10501        FSB T93
04031 -0 12000 0 04071        TMI XWS
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04032   0 56000 2 00004          LDQ 4,2
04033   0 26000 2 00011          FMP 9,2
04034   0 76500 0 00043          LRS 35
04035   0 26000 2 00011          FMP 9,2
04036   0 60100 0 10501          STO T93
04037   0 56000 2 00007          LDQ 7,2
04040   0 26000 2 00007          FMP 7,2
04041   0 76500 0 00043          LRS 35
04042   0 26000 2 00006          FMP 6,2
04043   0 30000 0 10501          FAD T93
04044   0 60100 0 10501          STO T93
04045   0 56000 2 00010          LDQ 8,2
04046   0 26000 2 00010          FMP 8,2
04047   0 76500 0 00043          LRS 35
04050   0 26000 2 00005          FMP 5,2
04051   0 30000 0 10501          FAD T93
04052   0 60100 0 10501          STO T93
04053   0 56000 2 00004          LDQ 4,2
04054   0 26000 2 00005          FMP 5,2
04055   0 76500 0 00043          LRS 35
04056   0 26000 2 00006          FMP 6,2
04057   0 30200 0 10501          FSB T93
04060   0 60100 0 10501          STO T93
04061   0 56000 2 00007          LDQ 7,2
04062   0 26000 2 00010          FMP 8,2
04063   0 76500 0 00043          LRS 35
04064   0 26000 2 00011          FMP 9,2
04065   0 76500 0 00043          LRS 35
04066   0 26000 0 04753          FMP C81
04067   0 30000 0 10501          FAD T93
04070   0 12000 0 04101          TPL XWT
04071   0 07400 4 06147  XWS     TSX OUT,4
04072   0 07400 4 05254          TSX ECHO,4
04073   3 23514 0 04754          PTH C82,0,10060
04074  -0 00036 0 10453          FOR T71,0,30
04075   1 00000 0 00003          PON U2,0,0
04076  -1 00000 0 00364          FVE 244
04077   0 50000 0 04336          CLA I1
04100   0 60100 0 10500          STO T92
04101  -2 00001 1 04110  XWT     TNX XVGG,1,1
04102   2 00000 2 04104  XWU     TIX XWV,2,0          DECREMENT TO BE SET
04103   0 00000 0 00144          HTR RCD
04104   0 50000 0 10453  XWV     CLA T71
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04105   0 40000 0 04336          ADD I1
04106   0 60100 0 10453          STO T71
04107   0 02000 0 03772          TRA XWP
04110   0 50000 0 10500  XVGG    CLA T92
04111  -0 10000 0 04115          TNZ XVGG1
04112   0 76000 0 00164          SWT 4
04113   0 02000 0 04115          TRA XVGG1
04114   0 02000 0 04120          TRA XVH
04115   0 07400 4 06147  XVGG1   TSX OUT,4
04116   0 07400 4 05254          TSX ECHO,4
04117  -1 00000 0 00361          FVE 241
04120   0 77200 0 00204  XVH     REW U1
04121   0 77200 0 00205  XVI     REW U3                  OR TRA XVJ
04122   0 07400 4 00146          TSX WTB,4
04123   0 00000 0 00005          PZE U3
04124   0 00000 0 77323  XVI1    PZE -START,0,0          DECREMENT TO BE SET
04125   0 76200 0 00225          RTB U3
04126   0 07400 4 00146          TSX WTB,4
04127   0 00000 0 00005          PZE U3
04130   0 00000 0 00400          PZE -32512,0,0
04131   0 77200 0 00205          REW U3
04132   0 50000 0 10500  XVJ     CLA T92
04133   0 10000 0 00160          TZE KH
04134   0 02000 0 00161          TRA KI
                                     SENSE-SETTING WORDS
04135   0 02000 0 10526          TRA XD1
04136   0 76100 0 00000  1XD     NOP
04137   0 02000 0 01070          TRA XH
04140   0 60000 0 10333  1XF     STZ T12
04141   0 00000 0 00001          PZE 1
04142   0 00000 0 00002          PZE 2
04143   0 00000 0 00001  1S3     PZE 1
04144   0 02000 0 03776          TRA XWQ
04145   0 50000 2 00004  1XWP1   CLA 4,2
04146   0 02000 0 03754          TRA XWH
04147   0 50000 0 10477  1XWD    CLA T91
04150   0 50000 0 04337          CLA I2
04151   0 02000 0 00621          TRA XCE
04152   0 02000 0 00621  1XGA    TRA XCE
04153   0 02000 0 00660          TRA XCG
04154   0 50000 0 05025  1XCF    CLA C90
04155   0 02000 0 03164          TRA XSB
04156   0 77000 0 00205  1XSA    WEF U3
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```
      04157  0 76200 0 00321  2XSB   RCD
      04160  0 02000 0 04120  1XSB   TRA  XVH
TD    04161  1 00000 0 01415         TXI  XAK
TD    04162  1 00000 0 01354  1XAH   TXI  XAI
TD    04163  1 00000 0 01541         TXI  XAW3
      04164  0 56000 0 10520  1XAW1  LDQ  M12
      04165  1 77773 2 03105         TXI  XFF3,2,-5
      04166  1 77773 2 03115  1XFF2  TXI  XFG,2,-5
      04167  0 53400 1 04340         LXA  I3,1
TD    04170  1 00000 0 01070  1XG    TXI  XH
      04171  0 53400 4 04343         LXA  I6,4
      04172  1 77777 2 01135  1XJ    TXI  XK,2,-1
      04173  0 53400 4 04343         LXA  I6,4
      04174  1 77777 1 01157  1XM    TXI  XN,1,-1
      04175  0 53400 4 04343         LXA  I6,4
      04176  1 77777 1 01201  1XP    TXI  XQ,1,-1
      04177  1 77766 2 01240         TXI  XW,2,-10
      04200  0 56000 0 10513  1XV    LDQ  M7
TD    04201  1 00000 0 01273         TXI  XAA
      04202  0 56000 0 10356  1XZ    LDQ  T31
TD    04203  1 00000 0 01327         TXI  XAE
      04204  0 56000 0 10357  1XAD   LDQ  T32
      04205  0 00000 0 00012         PZE  10
      04206  0 00000 0 00005  1T41   PZE  5
      04207  0 02000 0 00725         TRA  XA
      04210  0 60000 0 05362         STZ  SWTF8
      04211  0 60000 0 05362  1XCH   STZ  SWTF8
TD    04212  1 00000 0 02035         TXI  XBH
      04213  0 50000 0 10377         CLA  T48
      04214  0 50000 0 10377  1XAY   CLA  T48
TD    04215  1 00000 0 02035         TXI  XBH
TD    04216  1 00000 0 02035         TXI  XBH
TD    04217  1 00000 0 01740  1XBB1  TXI  XBG
TD    04220  1 00000 0 00725         TXI  XA
      04221  0 76600 0 00225  1XBH   WTB  U3
      04222  0 02000 0 04132         TRA  XVJ
      04223  0 77200 0 00205  1XVI   REW  U3
TD    04224  1 00000 0 02243         TXI  XBK
      04225  0 50000 0 10510  1XAW   CLA  M4
      04226  0 02000 0 03162         TRA  XSA
      04227  0 50000 0 10375  1XBI   CLA  T46
      04230 -2 00153 2 00000  2XFF1  MTW  0,2,107
      04231 -1 00153 2 00000  1XFF1  MON  0,2,107
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TD    04232  1 00000 0 01226  2XU1   TXI XU2
      04233 -0 76000 0 00003  1XU1   SSM
      04234  0 02000 0 03633  2XUO   TRA XUP
      04235 -0 50000 0 04735  1XUO   CAL C75
      04236  0 50000 0 10347         CLA T24
TD    04237  1 00000 0 01201  1XN    TXI XQ
      04240  0 56000 0 10354         LDQ T29
TD    04241  1 00000 0 01335  1XAB   TXI XAF
TD    04242  1 00000 0 01363         TXI XAJ
      04243  0 50000 0 10363  1XAI   CLA T36
TD    04244  1 00000 0 01435         TXI XAL
      04245  0 50000 0 10363  1XAK   CLA T36
      04246  0 56000 0 10366         LDQ T39
TD    04247  1 00000 0 01523  1XAR   TXI XAS
      04250  0 76100 0 00000         NOP
TD    04251  1 00000 0 01512  1XAV   TXI XAP
      04252  0 02000 0 01213         TRA XS2
      04253  0 50000 0 04335  1XS1   CLA IO
TD    04254  1 00000 0 01717         TXI XAY
      04255  0 50000 0 10516  1XBK   CLA M10
TD    04256  1 00000 0 01157         TXI XN
      04257  0 53400 4 04340  1XL    LXA I3,4
TD    04260  1 00000 0 01201         TXI XQ
      04261  0 53400 4 04340  1XO    LXA I3,4
      04262  1 77777 1 01303         TXI XAB,1,-1
      04263  0 56000 0 10355  1XY    LDQ T30
      04264  1 77777 1 01335         TXI XAF,1,-1
      04265  0 56000 0 10355  1XAC   LDQ T30
TD    04266  1 00000 0 01533         TXI XAW
      04267  0 50000 0 10520  1XAM   CLA M12
TD    04270  1 00000 0 01533         TXI XAW
      04271  0 50000 0 10520  1XAN   CLA M12
      04272  0 70000 0 10516         CPY M10
      04273  0 70000 0 10516         CPY M10
TD    04274  1 00000 0 00725  1XBH4  TXI XA
      04275  0 70000 0 10521         CPY M13
TD    04276  1 00000 0 00725         TXI XA
TD    04277  1 00000 0 00725  1XBH5  TXI XA
      04300  3 37340 0 04446         PTH C27,0,16096
      04301  3 33404 0 04430         PTH C26,0,14084
      04302  3 21536 0 04417         PTH C25,0,9054
      04303  3 13624 0 04411  1XCH5  PTH C24,0,6036
      04304  0 02000 0 02014         TRA XBG6
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04305  0 02000 0 01773          TRA XBG4
04306  0 02000 0 01755          TRA XBG2
04307  0 07400 4 05336  1XBG    TSX SWTF,4
04310  3 13632 0 04513          PTH C35,0,6042
04311  3 15610 0 04504          PTH C34,0,7048
04312  3 07676 0 04500          PTH C33,0,4030
04313  3 13632 0 04472  1XEC1   PTH C32,0,6042
04314  3 03745 0 04524          PTH C38,0,2021
04315  3 01767 0 04523  1XEC2   PTH C37,0,1015
04316  3 21563 0 04741          PTH C79,0,9075
04317  3 03761 0 04534          PTH C41,0,2033
04320  3 03761 0 04532  1XEC3   PTH C40,0,2033
04321  3 01772 0 04543          PTH C45,0,1018
04322  3 03750 0 04541          PTH C44,0,2024
04323  3 01772 0 04540  1XEC4   PTH C43,0,1018
04324  3 05731 0 04560          PTH C49,0,3033
04325  3 07707 0 04554          PTH C48,0,4039
04326  3 11665 0 04547  1XEE1   PTH C47,0,5045
04327  3 03772 0 04572          PTH C52,0,2042
04330  3 03772 0 04570  1XEG1   PTH C51,0,2042
04331  3 03734 0 04615          PTH C57,0,2012
04332  3 05712 0 04612  1XEK1   PTH C56,0,3018
04333  3 13624 0 04642          PTH C62,0,6036
04334  3 11646 0 04635  1XEK2   PTH C61,0,5030
                                     INTEGERS
04335  0 00000 0 00000  I0      PZE 0
04336  0 00000 0 00001  I1      PZE 1
04337  0 00000 0 00002  I2      PZE 2
04340  0 00000 0 00003  I3      PZE 3
04341  0 00000 0 00004  I4      PZE 4
04342  0 00000 0 00005  I5      PZE 5
04343  0 00000 0 00006  I6      PZE 6
04344  0 00000 0 00007  I7      PZE 7
04345  0 00000 0 00010  I8      PZE 8
04346  0 00000 0 00011  I9      PZE 9
04347  0 00000 0 00013  I11     PZE 11
04350  0 00000 0 00014  I12     PZE 12
04351  0 00000 0 00044  I36     PZE 36
04352  000000000023     IC      BCD 100000C
04353  000000000042     IK      BCD 100000K
04354  000000000044     IM      BCD 100000M
04355  000000000047     IP      BCD 100000P
04356  000000000062     IS      BCD 100000S
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04357  000000000063     IT     BCD 100000T
                                CONSTANTS
04360 +201400000000     C1     OCT 201400000000       FLOATING ONE
04361 +203622077324     C2     DEC 6.2831853          2PI
04362  606060606060     C3     BCD 1                  INDICATORS FOR OUTPUT
04363  546060606060     C4     BCD 1*                 X
04364  545460606060     C5     BCD 1**                X
04365  547354546060     C6     BCD 1*,**              X
04366 +202400000000     C7     DEC 2.                 LIMIT ON DELTA/SIGMA
04367  606060006060     C9     BCD 2   0   0   0
04370  600060606000
04371  456444255121     C19    BCD 5NUMERATOR   DENOMINATOR      R
04372  634651606060
04373  242545464431
04374  452163465160
04375  606060606051
04376  605160262123     C20    BCD 2 R FACTOR
04377  634651606060
04400  606625312730     C21    BCD 3 WEIGHTED R FACTOR
04401  632524605160
04402  262123634651
04403  314523436424     C22    BCD 3INCLUDING ZEROS
04404  314527607125
04405  514662606060
04406  464431636331     C23    BCD 3OMITTING ZEROS
04407  452760712551
04410  466260606060
04411  606060306060     C24    BCD 6   H   K   L   CALCULATED         A
04412  604260606043
04413  606060232143
04414  236443216325
04415  246060606060
04416  606060602160
04417  606060306060     C25    BCD 9   H   K   L   CALCULATED         A             B
04420  604260606043
04421  606060232143
04422  236443216325
04423  246060606060
04424  606060602160
04425  606060606060
04426  606060606022
04427  606060606060
04430  606060306060     C26    BCD     H   K   L     OBSERVED   CALCULATED         A          OBS
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04431  604260606043
04432  606060606046
04433  226225516525
04434  246060602321
04435  432364432163
04436  252460606060
04437  606060606021
04440  606060606060
04441  606060462262
04442  402321436060            BCD 4-CAL  (OBS-CAL)/SIGMA
04443  744622624023
04444  214334616231
04445  274421606060
04446  606060306060      C27   BCD     H   K   L     OBSERVED   CALCULATED         A
04447  604260606043
04450  606060606046
04451  226225516525
04452  246060602321
04453  432364432163
04454  252460606060
04455  606060606021
04456  606060606060
04457  606060606060
04460  226060606060            BCD 6B         OBS-CAL  (OBS-CAL)/SIGMA
04461  606060604622
04462  624023214360
04463  607446226240
04464  232143346162
04465  312744216060
04466 -0 00147 0 10424  C28   MZE T58,0,103
04467 -1 00147 1 10321  C29   MON S1+12,1,103
04470 -0 00457 0 00000  C30   MZE 0,0,303
04471  604446242540     C31   BCD 1 MODE-
04472  602346444764     C32   BCD 6 COMPUTE FIXED ATOM CONTRIBUTIONS
04473  632560263167
04474  252460216346
04475  446023464563
04476  513122646331
04477  464562606060
04500  602346444764     C33   BCD 4 COMPUTE F OR F SQUARED
04501  632560266046
04502  516026606250
04503  642151252460
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04504  602346444764     C34   BCD 7 COMPUTE DERIVATIVES FOR LEAST SQUARES
04505  632560242551
04506  316521633165
04507  256260264651
04510  604325216263
04511  606250642151
04512  256260606060
04513  604325216263     C35   BCD 6 LEAST SQUARES USING OLD DERIVATIVES
04514  606250642151
04515  256260646231
04516  452760464324
04517  602425513165
04520  216331652562
04521  602221622524     C36   BCD 2 BASED ON
04522  604645606060
04523  602660606060     C37   BCD 1 F
04524  602660625064     C38   BCD 2 F SQUARED
04525  215125246060
04526  606325444725     C39   BCD 4 TEMPERATURE FACTORS-
04527  512163645125
04530  602621236346
04531  516240606060
04532  606270444425     C40   BCD 2 SYMMETRIC
04533  635131236060
04534  602145316246     C41   BCD 2 ANISOTROPIC
04535  635146473123
04536  602223246046     C42   BCD 2 BCD OUTPUT-
04537  646347646340
04540  602664434360     C43   BCD 1 FULL
04541  604721516331     C44   BCD 2 PARTIAL
04542  214360606060
04543  604546452560     C45   BCD 1 NONE
04544  602231452151     C46   BCD 3 BINARY OUTPUT-
04545  706046646347
04546  646340606060
04547  606330516460     C47   BCD 5 THRU FIXED ATOM CONTRIBUTIONS
04550  263167252460
04551  216346446023
04552  464563513122
04553  646331464562
04554  606330516460     C48   BCD 4 THRU F OR F SQUARED
04555  266046516026
04556  606250642151
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04557  252460606060
04560  606330516460      C49   BCD 3 THRU DERIVATIVES
04561  242551316521
04562  633165256260
04563  604622622551      C50   BCD 5 OBSERVED F OR F SQUARED TO BE
04564  652524602660
04565  465160266062
04566  506421512524
04567  606346602225
04570  602346456231      C51   BCD 2 CONSIDERED
04571  242551252460
04572  603127454651      C52   BCD 2 IGNORED
04573  252460606060
04574  604525646351      C53   BCD 2 NEUTRON
04575  464560606060
04576  606740512170      C54   BCD 6 X-RAY WITH    KINDS OF FORM FACTORS
04577  606631633060
04600  606060423145
04601  246260462660
04602  264651446026
04603  212363465162
04604  604564442225      C55   BCD 6 NUMBER OF ATOMS IN ASYMMETRIC UNIT-
04605  516046266021
04606  634644626031
04607  456021627044
04610  442563513123
04611  606445316340
04612  602325456351      C56   BCD 3 CENTROSYMMETRIC
04613  466270444425
04614  635131236060
04615  602123254563      C57   BCD 2 ACENTRIC
04616  513123606060
04617  604564442225      C58   BCD 8 NUMBER OF SYMMETRY CARDS OR SYMMETRY ROUTINES-
04620  516046266062
04621  704444256351
04622  706023215124
04623  626046516062
04624  704444256351
04625  706051466463
04626  314525624060
04627  604564442225      C59   BCD 5 NUMBER OF SCALE FACTORS-
04630  516046266062
04631  232143256026
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04632  212363465162
04633  406060606060
04634  0 00000 0 00017  C60   PZE 15                    MASK USED TO DECODE SYMMETRY CARDS
04635  606462256027     C61   BCD 5 USE GENERAL SYMMETRY ROUTINE
04636  254525512143
04637  606270444425
04640  635170605146
04641  646331452560
04642  606270444425     C62   BCD 6 SYMMETRY ROUTINES SUPPLIED BY USER
04643  635170605146
04644  646331452562
04645  606264474743
04646  312524602270
04647  606462255160
04650  606250642151     C63   BCD   SQUARE ROOT (SUM W(OBS-CALC)**2/(M-N))                    S
04651  256051464663
04652  607462644460
04653  667446226240
04654  232143233454
04655  540261744440
04656  453434606060
04657  606060606060
04660  606060606060
04661  606060606062
04662  505163746060           BCD 3QRT(   0-  0)
04663  600040606000
04664  346060606060
04665  0 00000 0 77760  C64   PZE K1                   ADDRESS OF FIRST INTERSEGMENT TEMPORARY
04666  604721512144     C65   BCD   PARAMETER            OLD       CHANGE        NEW        ERROR
04667  256325516060
04670  606060606060
04671  606046432460
04672  606060606023
04673  302145272560
04674  606060606060
04675  452566606060
04676  606060602551
04677  514651606060
04700  622321432560     C66   BCD 2SCALE FACTOR
04701  262123634651
04702  466525512143     C67   BCD 2OVERALL B
04703  436022606060
04704  602163464460     C68   BCD 1 ATOM
```

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04705  602646514460      C69   BCD 2 FORM FACTOR
04706  262123634651
04707  606760606060            BCD 2 X
04710  606060606060
04711  607060606060            BCD 2 Y
04712  606060606060
04713  607160606060            BCD 2 Z
04714  606060606060
                 04715  C70    BSS 2                    TO BE SET
04717  602225632174            BCD 2 BETA(2,2)
04720  027302346060
04721  602225632174            BCD 2 BETA(3,3)
04722  037303346060
04723  602225632174            BCD 2 BETA(1,2)
04724  017302346060
04725  602225632174            BCD 2 BETA(1,3)
04726  017303346060
04727  602225632174            BCD 2 BETA(2,3)
04730  027303346060
04731  602163464431      C71   BCD 2 ATOMIC B
04732  236022606060
04733  602225632174      C72   BCD 2 BETA(1,1)
04734  017301346060
04735 -0 00025 1 00000   C75   FOR 0,1,21              X-RAY FORM FACTOR OUTPUT
04736 -3 15561 1 00000   C76   SVN 0,1,7025            NEUTRON FORM FACTOR OUTPUT
04737  0 00026 0 00000   C77   PZE 0,0,22
04740  0 00000 0 04705   C78   PZE C69                  ADDRESS OF FIRST TITLE
04741  606270444425      C79   BCD 9 SYMMETRIC CONVERTED TO ANISOTROPIC BEFORE REFINING
04742  635131236023
04743  464565255163
04744  252460634660
04745  214531624663
04746  514647312360
04747  222526465125
04750  605125263145
04751  314527606060
04752 +177400000000      C80   DEC .25
04753 +202400000000      C81   DEC 2.
04754  606325444725      C82   BCD   TEMPERATURE FACTOR OF ATOM    IS NOT POSITIVE-DEFINITE.
04755  512163645125
04756  602621236346
04757  516046266021
04760  634644606060
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04761  603162604546
04762  636047466231
04763  633165254024
04764  252631453163
04765  253360606060
04766  602431622351      C83   BCD 8 DISCREPANCY FACTORS BASED ON INPUT PARAMETERS.
04767  254721452370
04770  602621236346
04771  516260222162
04772  252460464560
04773  314547646360
04774  472151214425
04775  632551623360
04776  602562633144      C84   BCD 2 ESTIMATE OF
04777  216325604626
05000  602221622524      C85   BCD 5 BASED ON OUTPUT PARAMETERS.
05001  604645604664
05002  634764636047
05003  215121442563
05004  255162336060
05005  606364514560      C86   BCD   TURN ON SENSE SWITCH   TO SUPPRESS ON-LINE PRINTING OF
05006  464560622545
05007  622560626631
05010  632330606060
05011  634660626447
05012  475125626260
05013  464540433145
05014  256047513145
05015  633145276046
05016  266060606060
05017  472151214425      C87   BCD 2PARAMETERS.
05020  632551623360
05021  266046516026      C88   BCD 3F OR F SQUARED.
05022  606250642151
05023  252433606060
05024  0 00000 0 00020   C89   PZE 16                 NO. OF INTERSEGMENT STORAGE LOCATIONS
05025  3 77777 7 77323   C90   PTH -START,7,32767     USED TO COMPUTE LENGTH OF DUMMY RECORD
05026  0 00000 0 00300   C91   PZE 192                LENGTH OF DUMMY RECORD 3
05027  0 00000 0 00200   C92   PZE 128                LENGTH OF DUMMY RECORD 4
                                 SUBROUTINE TO CHECK IDENTIFICATION LETTER
05030  0 76000 0 00166   IFF   SWT 6
05031  0 02000 0 05033         TRA IFF1
05032  0 02000 4 00003         TRA 3,4
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```
05033  0 50000 4 00001  IFF1  CLA 1,4
05034  0 62100 0 05040        STA IFF2
05035  0 77100 0 00022        ARS 18
05036  0 62100 0 05043        STA IFF3
05037  0 62100 0 05056        STA IFF6
05040  0 50000 0 00000  IFF2  CLA 0                  ADDRESS TO BE SET
05041 -0 32000 0 05133        ANA IFF11
05042  0 60100 0 05134        STO IFF12
05043  0 34000 0 00000  IFF3  CAS 0                  ADDRESS TO BE SET
05044  1 00000 0 05046  IFF4  TXI IFF5,0,0
05045  0 02000 4 00003        TRA 3,4
05046 -0 63400 4 05044  IFF5  SXD IFF4,4
05047  0 07400 4 06147        TSX OUT,4
05050  0 07400 4 05254        TSX ECHO,4
05051  3 02015 0 05134        PTH IFF12,0,1037
05052  3 13624 0 05076        PTH IFF7,0,6036
05053 -1 00000 0 00364        FVE 244
05054  0 07400 4 06147        TSX OUT,4
05055  0 07400 4 05254        TSX ECHO,4
05056  3 02015 0 00000  IFF6  PTH 0,0,1037           ADDRESS TO BE SET
05057  3 13624 0 05104        PTH IFF8,0,6036
05060 -1 00000 0 00364        FVE 244
05061  0 07400 4 06147        TSX OUT,4
05062  0 07400 4 05254        TSX ECHO,4
05063  3 15602 0 05112        PTH IFF9,0,7042
05064 -1 00000 0 00364        FVE 244
05065  0 07400 4 06147        TSX OUT,4
05066  0 07400 4 05254        TSX ECHO,4
05067  3 23514 0 05121        PTH IFF10,0,10060
05070 -1 00000 0 00364        FVE 244
05071  0 07400 4 06147        TSX OUT,4
05072  0 07400 4 05254        TSX ECHO,4
05073 -1 00000 0 00361        FVE 241
05074 -0 53400 4 05044        LXD IFF4,4
05075  0 00000 4 00002        HTR 2,4
05076  602421632160     IFF7  BCD 6 DATA CARD IDENTIFICATION LETTER IS
05077  232151246031
05100  242545633126
05101  312321633146
05102  456043256363
05103  255160316260
05104  604751462751     IFF8  BCD 6 PROGRAM CALLS FOR CARD WITH LETTER
05105  214460232143
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05106  436260264651
05107  602321512460
05110  663163306043
05111  256363255160
05112  604764636023      IFF9  BCD 7 PUT CORRECT CARD IN READER AND PROCEED.
05113  465151252363
05114  602321512460
05115  314560512521
05116  242551602145
05117  246047514623
05120  252524336060
05121  606346602270      IFF10 BCD   TO BYPASS ALL IDENTIFICATION TESTS TURN ON SENSE SWITCH 6.
05122  472162626021
05123  434360312425
05124  456331263123
05125  216331464560
05126  632562636260
05127  636451456046
05130  456062254562
05131  256062663163
05132  233060063360
05133  0 00000 0 00177  IFF11 PZE 127                    MASK
05134  0 00000 0 00000  IFF12                            LETTER FROM CARD
                                SUBROUTINE TO TEST FOR BLANK FIELD
05135 -0 63400 1 05143  BLNK  SXD BLNK2,1
05136  0 50000 4 00001        CLA 1,4
05137  0 62100 0 05141        STA BLNK1
05140 -0 73400 1 00000        PDX 0,1
05141  0 50000 1 00000  BLNK1 CLA 0,1                    ADDRESS TO BE SET
05142  0 34000 0 05152        CAS BLNK5
05143  1 00000 0 05145  BLNK2 TXI BLNK3,0,0
05144  0 02000 0 05147        TRA BLNK4
05145 -0 53400 1 05143  BLNK3 LXD BLNK2,1
05146  0 02000 4 00003        TRA 3,4
05147  2 00001 1 05141  BLNK4 TIX BLNK1,1,1
05150 -0 53400 1 05143        LXD BLNK2,1
05151  0 02000 4 00002        TRA 2,4
05152  606060606060     BLNK5 BCD 1
                                OCTAL AND FLOATING DECIMAL DUMP FOR TEST PURPOSES
05153  0 07400 4 06147  DUMP  TSX OUT,4
05154  0 07400 4 05254        TSX ECHO,4
05155  3 27451 0 10406        PTH T55,0,12073
05156  3 02066 0 04362        PTH C3,0,1078
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05157  1 00001 0 00003          PON U2,0,1
05160  0 53400 1 05252          LXA DUMP7,1
05161  0 07400 4 06147  DUMP1   TSX OUT,4
05162  0 07400 4 05254          TSX ECHO,4
05163 -2 17531 1 00000          SIX 0,1,8025
05164 -2 17562 1 00001          SIX 1,1,8050
05165 -2 17613 1 00002          SIX 2,1,8075
05166 -2 17644 1 00003          SIX 3,1,8100
05167  1 00000 0 00003          PON U2,0,0
05170 -0 75400 1 00000          PXD 0,1
05171  0 77100 0 00022          ARS 18
05172  0 76000 0 00006          COM
05173  0 40000 0 04336          ADD I1
05174  0 73400 2 00000          PAX 0,2
05175 -0 75400 2 00000          PXD 0,2
05176  0 76500 0 00043          LRS 35
05177  0 53400 4 04343          LXA I6,4
05200  0 76700 0 00003  DUMP8   ALS 3
05201 -0 76300 0 00003          LGL 3
05202  2 00001 4 05200          TIX DUMP8,4,1
05203 -0 50100 0 05253          ORA DUMP9
05204  0 60200 0 05251          SLW DUMP6+8
05205  0 53400 2 04345          LXA I8,2
05206  0 56000 1 00000  DUMP2   LDQ 0,1
05207  0 53400 4 04343          LXA I6,4
05210  0 76700 0 00003  DUMP3   ALS 3
05211 -0 76300 0 00003          LGL 3
05212  2 00001 4 05210          TIX DUMP3,4,1
05213  0 60200 2 05251          SLW DUMP6+8,2
05214  0 53400 4 04343          LXA I6,4
05215  0 76700 0 00003  DUMP4   ALS 3
05216 -0 76300 0 00003          LGL 3
05217  2 00001 4 05215          TIX DUMP4,4,1
05220  0 60200 2 05252          SLW DUMP6+9,2
05221  1 77777 1 05222          TXI DUMP5,1,-1
05222  2 00002 2 05206  DUMP5   TIX DUMP2,2,2
05223  0 07400 4 06147          TSX OUT,4
05224  0 07400 4 05254          TSX ECHO,4
05225  3 01756 0 05251          PTH DUMP6+8,0,1006
05226  3 01772 0 05241          PTH DUMP6,0,1018
05227  3 02001 0 05242          PTH DUMP6+1,0,1025
05230  3 02023 0 05243          PTH DUMP6+2,0,1043
05231  3 02032 0 05244          PTH DUMP6+3,0,1050
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05232  3 02054 0 05245          PTH DUMP6+4,0,1068
05233  3 02063 0 05246          PTH DUMP6+5,0,1075
05234  3 02105 0 05247          PTH DUMP6+6,0,1093
05235  3 02114 0 05250          PTH DUMP6+7,0,1100
05236  1 00060 0 00003          PON U2,0,48
05237  3 66653 1 05161          TXH DUMP1,1,-T5-256   DECREMENT IS -(FINAL ADDRESS+1)
05240  0 02000 0 00144          TRA RCD
                 05241  DUMP6 BSS 9
05252  0 00000 0 67473  DUMP7 PZE -S1                -(INITIAL ADDRESS)
05253  600000000000     DUMP9 BCD 1 00000
                                 SUBROUTINE TO TEST NATURE OF ERROR RETURN FROM NY OUT3
05254  0 12000 0 05272  ECHO  TPL ECHO4
05255 -0 10000 0 05272          TNZ ECHO4
05256 -0 63400 4 05310          SXD ECHO7,4
05257  0 07400 4 06147          TSX OUT,4
05260  0 02000 0 05263          TRA ECHO2
05261  3 15602 0 05301          PTH ECHO6,0,7042
05262 -1 00000 0 00000  ECHO1 FVE
05263 -0 53400 4 05310  ECHO2 LXD ECHO7,4
05264 -0 50000 4 00001  ECHO3 CAL 1,4
05265  0 77100 0 00041          ARS 33
05266  0 34000 0 05300          CAS ECHO5
05267  1 77777 4 05264          TXI ECHO3,4,-1
05270  0 02000 4 00002          TRA 2,4               TO NORMAL RETURN OF NY OUT3
05271  1 77777 4 05264          TXI ECHO3,4,-1
05272 -0 75400 4 00000  ECHO4 PXD 0,4
05273  0 76000 0 00006          COM
05274 -0 73400 4 00000          PDX 0,4
05275 -0 75400 4 00000          PXD 0,4
05276  0 77100 0 00022          ARS 18
05277  0 00000 0 00144          HTR RCD               CALLING SEQUENCE ERROR. ADDRESS IN ACC.
05300  0 00000 0 00005  ECHO5 PZE 5
05301  605454546047     ECHO6 BCD 7 *** PRINTER ERROR IN PREVIOUS LINE ***
05302  513145632551
05303  602551514651
05304  603145604751
05305  256531466462
05306  604331452560
05307  545454606060
05310  0 00000 0 00000  ECHO7 PZE                     INDEX SAVED IN DECREMENT
                                 SUBROUTINE TO SUPPRESS ON-LINE PRINTING OF PARAMETERS
05311  0 50000 4 00001  SWTP  CLA 1,4
05312  0 62100 0 05331          STA SWTP5
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05313  0 76000 0 00164          SWT  4
05314  0 02000 0 05327          TRA  SWTP4
05315  0 50000 0 05335          CLA  SWTP8
05316  0 10000 0 05325          TZE  SWTP2
05317  0 60000 0 05335          STZ  SWTP8
05320 -0 63400 4 05326          SXD  SWTP3,4
05321  0 07400 4 06147  SWTP1   TSX  OUT,4
05322  0 07400 4 05254          TSX  ECHO,4
05323 -1 00000 0 00361          FVE  241
05324 -0 53400 4 05326          LXD  SWTP3,4
05325  0 56000 0 05333  SWTP2   LDQ  SWTP6
05326  1 00000 0 05331  SWTP3   TXI  SWTP5,0,0          INDEX SAVED IN DECREMENT
05327  0 56000 0 05334  SWTP4   LDQ  SWTP7
05330 -0 60000 0 05335          STQ  SWTP8
05331 -0 62000 0 00000  SWTP5   SLQ  0                  ADDRESS TO BE SET
05332  0 02000 4 00002          TRA  2,4
05333  0 76100 0 00000  SWTP6   NOP                    CONSTANT
05334 -1 00000 0 00000  SWTP7   FVE                    CONSTANT
05335  0 00000 0 00000  SWTP8   PZE                    INDICATOR
                                SUBROUTINE TO SUPPRESS ON-LINE PRINTING OF F OR F**2
05336  0 50000 4 00001  SWTF    CLA  1,4
05337  0 62100 0 05356          STA  SWTF5
05340  0 76000 0 00163          SWT  3
05341  0 02000 0 05354          TRA  SWTF4
05342  0 50000 0 05362          CLA  SWTF8
05343  0 10000 0 05352          TZE  SWTF2
05344  0 60000 0 05362          STZ  SWTF8
05345 -0 63400 4 05353          SXD  SWTF3,4
05346  0 07400 4 06147  SWTF1   TSX  OUT,4
05347  0 07400 4 05254          TSX  ECHO,4
05350 -1 00000 0 00361          FVE  241
05351 -0 53400 4 05353          LXD  SWTF3,4
05352  0 56000 0 05360  SWTF2   LDQ  SWTF6
05353  1 00000 0 05356  SWTF3   TXI  SWTF5,0,0          INDEX SAVED IN DECREMENT
05354  0 56000 0 05361  SWTF4   LDQ  SWTF7
05355 -0 60000 0 05362          STQ  SWTF8
05356 -0 62000 0 00000  SWTF5   SLQ  0                  ADDRESS TO BE SET
05357  0 02000 4 00002          TRA  2,4
05360  0 76100 0 00000  SWTF6   NOP                    CONSTANT
05361 -1 00000 0 00000  SWTF7   FVE                    CONSTANT
05362  0 00000 0 00000  SWTF8   PZE                    INDICATOR
                                THE FOLLOWING SUBROUTINES ARE ON RELOCATABLE CARDS
                     05363  DBD1   BSS  136
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                 05573  FILE   BSS 197
                 06100 BUFFER  BSS 14
                 06116  SQRT   BSS 25
                 06147  OUT    BSS 408
                 06777  SIN    BSS 24
                 07027  EXP    BSS 35
                 07072 TABLES  BSS 651
                                   SENSE INDICATORS
10305  0 00000 0 00000  S1                          MODE INDICATOR
10306  0 00000 0 00001  S2     PZE 1                F OR F SQUARED INDICATOR
10307  0 00000 0 00001  S3     PZE 1                SYMM OR ANIS INDICATOR
10310  0 00000 0 00001  S4     PZE 1                BCD OUTPUT INDICATOR
10311  0 00000 0 00002  S5     PZE 2                BINARY OUTPUT YES OR NO
10312  0 00000 0 00001  S6     PZE 1                OBSERVED TO BE CONSIDERED
10313  0 00000 0 00000  S7                          NUMBER OF FORM FACTOR TABLES
10314  0 00000 0 00000  S8                          NUMBER OF ATOMS IN ASYMMETRIC UNIT
10315  0 00000 0 00000  S9                          CENTRO OR ACENTRIC
10316  0 00000 0 00000  S10                         NO. OF SYMM CARDS OR SYMM ROUTINES
10317  0 00000 0 00001  S15    PZE 1                GENERAL OR USERS SYMMETRY ROUTINE
10320  0 00000 0 00001  S11    PZE 1                NO. OF SCALE FACTORS
10321  0 00000 0 00000  S12                         FIXED ATOM CONTRIBUTION INDICATOR
10322  0 00000 0 00000  S13                         ARE DERIVATIVES COMPUTED
10323  0 00000 0 00000  S14                         EXTENT OF BINARY OUTPUT
                                   TEMPORARY STORAGE
                 10316  T1     SYN S10
                 10314  T2     SYN S8
                 10320  T3     SYN S11
                 10313  T4     SYN S7
10324  0 00000 0 00000  T61                         COMP LOC FIRST SYMMETRY CODE WORD
10325  0 00000 0 00000  T6                          COMP LOC FIRST ATOM PARAMETER
10326  0 00000 0 00000  T7                          COMP LOC SUMMATION STORAGE
10327  0 00000 0 00000  T8                          COMP LOC DERIVATIVE STORAGE
10330  0 00000 0 00000  T11                         COMP LOC FORM FACTOR STORAGE
10331  0 00000 0 00000  T9                          NO. OF ATOMIC PARAMETERS
10332  0 00000 0 00000  T10                         NO. OF INTERMEDIATE SUMS
10333  0 00000 0 00000  T12                         T(J)
10334  0 00000 0 00000  T13                         H(J)
10335  0 00000 0 00000  T14                         K(J)
10336  0 00000 0 00000  T15                         L(J)
10337  0 00000 0 00000  T16                         H**2(J)
10340  0 00000 0 00000  T17                         K**2(J)
10341  0 00000 0 00000  T18                         L**2(J)
10342  0 00000 0 00000  T19                         2HK(J)
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10343  0 00000 0 00000  T20                    2HL(J)
10344  0 00000 0 00000  T21                    2KL(J)
10345  0 00000 0 00000  T22                    TRIG ARGUMENT (I,J)
10346  0 00000 0 00000  T23                    INDEX I IN DECREMENT
10347  0 00000 0 00000  T24                    SIN(I,J), EXP(I,J)SIN(I,J)
10350  0 00000 0 00000  T25                    COS(I,J), EXP(I,J)COS(I,J)
10351  0 00000 0 00000  T26                    EXP ARGUMENT (I,J)
10352  0 00000 0 00000  T27                    EXP(I,J)
10353  0 00000 0 00000  T28                    INDEX J IN DECREMENT
10354  0 00000 0 00000  T29                    F(I), SYM T.F.(I)F(I)
10355  0 00000 0 00000  T30                    SYM T.F.(I)
10356  0 00000 0 00000  T31                    F(I)SYM T.F.(I)SUM(I)EXP(I,J)COS(I,J)
10357  0 00000 0 00000  T32                    F(I)SYM T.F.(I)SUM(I)EXP(I,J)SIN(I,J)
10360  0 00000 0 00000  T33                    2PI F(I)SYM T.F.(I)
10361  0 00000 0 00000  T34                    MINUS 2PI F(I)SYM T.F.(I)
10362  0 00000 0 00000  T35                    MINUS F(I)SYM T.F.(I)
10363  0 00000 0 00000  T36                    OVERALL T.F., SCALE*OV.T.F
10364  0 00000 0 00000  T37                    SCALE FACTOR
10365  0 00000 0 00000  T38                    COEFFICIENT OF D A/D PARAMETER
10366  0 00000 0 00000  T39                    COEFFICIENT OF D B/D PARAMETER
10367  0 00000 0 00000  T40                    A**2, (A**2+B**2)**(1/2),A**2+B**2
10370  0 00000 0 00000  T41                    5 FOR SYM OR 10 FOR ANIS T.F.
10371  0 00000 0 00000  T42                    R FACTOR NUMERATOR
10372  0 00000 0 00000  T43                    SAME OMITTING UNOBSERVEDS
10373  0 00000 0 00000  T44                    WEIGHTED R FACTOR NUMERATOR
10374  0 00000 0 00000  T45                    SAME OMITTING UNOBSERVEDS
10375  0 00000 0 00000  T46                    R FACTOR DENOMINATOR
10376  0 00000 0 00000  T47                    WEIGHTED R FACTOR DENOMINATOR
10377  0 00000 0 00000  T48                    (OBS-CALC)/SIGMA
10400  0 00000 0 00000  T49                    W*OBS**2
10401  0 00000 0 00000  T50                    HOLLERITH DISAGREEMENT INDICATOR
10402  0 00000 0 00000  T51                    R FACTOR
10403  0 00000 0 00000  T52                    SAME OMITTING UNOBSERVEDS
10404  0 00000 0 00000  T53                    WEIGHTED R FACTOR
10405  0 00000 0 00000  T54                    SAME OMITTING UNOBSERVEDS
                  10406  T55   BSS 12          IDENTIFICATION OF PROBLEM
10422  0 00000 0 00000  T56                    INDEX 4 IN DECREMENT
10423  0 00000 0 00000  T57                    W(OBS-CALC)**2
10424  0 00000 0 00000  T58                    SENSE INPUT TO TEST FOR BLANK
10425  0 00000 0 00000  T59                    MACHINE CAPACITY LESS ONE
                  10426  T60   BSS 6           COMPONENTS OF TRANSFORMED INDICES
10434  0 00000 0 00000  T62                    COMP CURRENT LOC SYMM CODE WORD
                  10435  T63   BSS 6           HOLLERITH INPUT FROM SYMMETRY CARDS
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10443   0 00000 0 00000   T64                          NUMBER OF SYMMETRY CODE WORDS
10444   0 00000 0 00000   T65                          M, NUMBER OF REFLECTIONS USED
10445   0 00000 0 00000   T66                          SUM W(OBS-CALC)**2 FOR REFLECTIONS USED
10446   0 00000 0 00000   T67                          N, NUMBER OF PARAMETERS VARIED
10447   0 00000 0 00000   T68                          SQRT (SUM W(OBS-CALC)**2/(M-N))
10450   0 00000 0 00000   T69                          DISCARDS COPIED HERE
                  10451   T70    BSS 2                 PARAMETER TITLE FOR OUTPUT
10453   0 00000 0 00000   T71                          SCALE FACTOR OR ATOM NUMBER
10454   0 00000 0 00000   T72                          OLD PARAMETER
10455   0 00000 0 00000   T73                          NEW PARAMETER
10456   0 00000 0 00000   T74                          STANDARD ERROR OF PARAMETER
10457   0 00000 0 00000   T75                          INDEX P IN DECREMENT
10460   0 00000 0 00000   T76                          INDEX I IN DECREMENT
10461   0 00000 0 00000   T77                          INDEX Q IN DECREMENT
10462   0 00000 0 00000   T78                          A*
10463   0 00000 0 00000   T79                          B*
10464   0 00000 0 00000   T80                          C*
10465   0 00000 0 00000   T81                          COS GAMMA*
10466   0 00000 0 00000   T82                          COS BETA*
10467   0 00000 0 00000   T83                          COS ALPHA*
10470   0 00000 0 00000   T84                          (.25)(A*)(A*)
10471   0 00000 0 00000   T85                          (.25)(B*)(B*)
10472   0 00000 0 00000   T86                          (.25)(C*)(C*)
10473   0 00000 0 00000   T87                          (.25)(A*)(B*)(COS GAMMA*)
10474   0 00000 0 00000   T88                          (.25)(A*)(C*)(COS BETA*)
10475   0 00000 0 00000   T89                          (.25)(B*)(C*)(COS ALPHA*)
10476   0 00000 0 00000   T90                          5(NO. OF ATOMS)
10477   0 00000 0 00000   T91                          B(I), OVERALL B
10500   0 00000 0 00000   T92                          INDICATOR FOR POS-DEF TEMP. FACTOR
10501   0 00000 0 00000   T93                          USED FOR TESTS ON TEMP. FACTORS
10502   0 00000 0 00000   T94                          CORRECTION TO SUM W(OBS-CALC)**2
10503   0 00000 0 00000   T95                          SQRT (SUM W(OBS-CALC)**2)
10504   0 00000 0 00000   T96                          HALF LENGTH OF CODE DUMP
                                     DATA AND OUTPUT TEMPORARIES
10505   0 00000 0 00000   M1                           H
10506   0 00000 0 00000   M2                           K
10507   0 00000 0 00000   M3                           L
10510   0 00000 0 00000   M4                           OBS
10511   0 00000 0 00000   M5                           SQRT W=1/SIGMA
10512   0 00000 0 00000   M6                           SCALE FACTOR IDENTIFICATION
10513   0 00000 0 00000   M7                           (SIN THETA/LAMBDA)**2
10514   0 00000 0 00000   M8                           FIXED ATOM A
10515   0 00000 0 00000   M9                           FIXED ATOM B
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10516   0 00000 0 00000   M10                          A
10517   0 00000 0 00000   M11                          B
10520   0 00000 0 00000   M12                          CALC
10521   0 00000 0 00000   M13                          OBS-CALC
10522   0 00000 0 00000   M14                          REJECTION INDICATOR
10523   0 00000 0 00000   M15                          D CALC/D SCALE
10524   0 00000 0 00000   M16                          D CALC/D OVERALL T.F.
                                     THE FOLLOWING MAY BE CHANGED BY THE USER
10525   0 00000 0 10526   T5     PZE XD1               ADDRESS OF LAST LOC USED
10526   0 00000 0 00000   XD1                          SYMMETRY ROUTINES IF WRITTEN BY USER
                                     IMMEDIATELY FOLLOWING THE ADDRESS SPECIFIED IN T5 THE
                                     PROGRAM ASSIGNS THE FOLLOWING STORAGE-
                                         SCALE FACTORS.
                                         OVERALL TEMPERATURE FACTOR.
                                         SIX SYMMETRY CODE WORDS FOR EACH SYMMETRY CARD.
                                         FIVE OR TEN PARAMETERS PER ATOM.
                                         FORM FACTORS UNLESS PROBLEM IS NEUTRON ONE.
                                         FIVE, TEN, OR TWENTY LOCATIONS PER ATOM USED
                                             FOR DERIVATIVES OF A AND B.
                                             THIS AREA LATER USED FOR PARAMETER CHANGES AND
                                             DIAGONAL ELEMENTS OF INVERSE MATRIX.
                                         FIVE OR TEN LOCATIONS PER ATOM USED FOR
                                             DERIVATIVES OF F OR F SQUARED.
                                     THE PROGRAM ASSIGNS THE FOLLOWING STORAGE
                                     IMMEDIATELY PRECEEDING INTERSEGMENT STORAGE-
                                         PARAMETER SELECTION WORDS.
                                     INTERSEGMENT TEMPORARY STORAGE
                     77760           ORG 32752
77760   0 00000 0 00000   K1                           NUMBER OF PARAMETER SELECTION WORDS
77761   0 00000 0 00000   K2                           NUMBER OF PARAMETERS TO BE VARIED
77762   0 00000 0 00000   K3                           NUMBER OF SCALE FACTORS TO BE VARIED
77763   0 00000 0 00000   K4                           NUMBER OF KINDS OF FORM FACTORS
77764   0 00000 0 00000   K5                           COMP. DERIV. ADDRESS IN DECREMENT
77765   0 00000 0 00000   K6                           BIT COUNTER IN DECREMENT
77766   0 00000 0 00000   K7                           SELECTION WORD COUNTER IN DECREMENT
77767   0 00000 0 00000   K8                           PARTLY SHIFTED SELECTION WORD
77770   0 00000 0 00000   K9                           BY-PASS INDICATOR
77771   0 00000 0 00000   K10                          COMP. INITIAL DERIVATIVE ADDRESS
77772   0 00000 0 00000   K11                          INITIAL MATRIX ADDRESS +N
77773   0 00000 0 00000   K12                          INITIAL VECTOR ADDRESS
77774   0 00000 0 00000   K13                          MODE NUMBER
77775   0 00000 0 00000   K14                          INITIAL MATRIX ADDRESS
77776   0 00000 0 00000   K15                          INITIAL SELECTION WORD ADDRESS
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77777   0 00000 0 00000  K16                          -MATRIX ADDRESS,0,-VECTOR ADDRESS
                                   THIS SECTION SUPPLIES ORIGIN CARDS FOR THE SUBROUTINES
                  00000          ORG 0
00000   0 00000 0 00000          PZE
00001   0 00000 0 05363          PZE DBD1
                  00000          ORG 0
00000   0 00000 0 00000          PZE
00001   0 00000 0 05573          PZE FILE
                  00000          ORG 0
00000   0 00000 0 00000          PZE
00001   0 00000 0 06116          PZE SQRT
                  00000          ORG 0
00000   0 00000 0 00000          PZE
00001   0 00000 0 06147          PZE OUT
                  00000          ORG 0
00000   0 00000 0 00000          PZE
00001   0 00000 0 06777          PZE SIN
                  00000          ORG 0
                                   MU SBL 2  0026 CARDS   SHIFTING BINARY LOADER-ONE CARD
00000   0 53400 4 00000  SBL2    LXA 0,4              CLEAR IR4
00001   0 70000 4 00002          CPY 2,4              COPYLOADER INTO 2,3, ETC.
00002   1 77777 4 00001          TXI 1,4,32767        REPEAT UNTIL LOADER IN
00003   0 00000 0 07072          HTR TABLES             SHIFTING INCREMENT
00004   0 76200 0 00321          RCD                  SELECT CARD READER
00005   0 70000 0 00000          CPY 0                9L IN O AND MQ
00006   0 76300 0 00021          LLS 17               WORD COUNT (=WC) IN AC ADDRESS
00007  -0 32000 0 00027          ANA 23               EXTRACT WORD COUNT
00010   0 70000 0 00001          CPY 1                9R IN 1 (CHECK SUM)
00011   0 10000 0 00000          TZE 0                IF WC=0, HAVE TRANSFER CARD, GO TO IT
00012   0 73400 4 00000          PAX 0,4              SET IR4=WC
00013   0 40000 0 00000          ADD 0                (WC+LA) IN AC (LA=LOAD ADDRESS)
00014   0 40000 0 00003          ADD 3                (WC+LA+INC) IN AC
00015   0 62100 0 00020          STA 16               PLANT (WC+LA+INC) AS CPY ADDRESS
00016   0 62100 0 00021          STA 17               AND AS ACL ADDRESS
00017  -0 50000 0 00000          CAL 0                PREPARE FOR CARD SUM
00020   0 70000 4 00000          CPY 0,4              COPY WORD FROM BINARY CARD
00021   0 36100 4 00000          ACL 0,4              AND ADD IT TO CARD SUM
00022   2 00001 4 00020          TIX 16,4,1           REPEATING UNTIL DONE
00023   0 60200 0 00002          SLW 2                FORM (CARD SUM)-(CHECK SUM)
00024   0 50000 0 00002          CLA 2                X
00025   0 40200 0 00001          SUB 1                X
00026   0 10000 0 00004          TZE 4                IF O, PROCEED TO NEXT CARD
00027   0 00000 0 00037          HTR 31               MASK FOR WORD COUNT (HALT FOR ERROR)
```

END 0

00000

```
                                        OR-XLS3   MATRIX STORING SEGMENT
                  00005  U3     EQU 5                  NUMBER OF BINARY OUTPUT TAPE
                  00144  RCD    EQU 100
                  00146  WTB    EQU 102
                  00455         ORG 301
00455  0 02000 0  00461  START  TRA XJA
00456  0 00000 0  00144         HTR RCD                NO ENTRY HERE
00457  0 02000 0  00144         TRA RCD
00460  0 00000 0  00144         HTR RCD                NO ENTRY HERE
00461  0 53400 4  77774  XJA    LXA K13,4
00462  3 00004 4  00464         TXH XJA1,4,4
00463  3 00002 4  00465         TXH XJA2,4,2
00464  0 00000 0  00144  XJA1   HTR RCD                INCORRECT MODE SPECIFIED
00465  0 50000 4  00717  XJA2   CLA 3XKL+3,4
00466  0 60100 0  00645         STO XKL
00467  0 53400 4  77770         LXA K9,4
00470  0 50000 4  00717         CLA 1XJK+1,4
00471  0 60100 0  00546         STO XJK
00472  0 50000 0  77775         CLA K14
00473  0 62100 0  00642         STA XKK2
00474  0 62100 0  00643         STA XKK3
00475  0 62100 0  00653         STA XKO
00476  0 62100 0  00654         STA XKO1
00477  0 62100 0  00674         STA XKT1
00500  0 50000 0  77776         CLA K15
00501  0 62100 0  00675         STA XKT2
00502  0 62100 0  00676         STA XKT3
00503  0 62100 0  00515         STA XJA3
00504  0 50000 0  77777         CLA K16
00505  0 76700 0  00022         ALS 18
00506  0 62200 0  00561         STD XJN1
00507  0 50000 0  77761         CLA K2
00510  0 40000 0  00720         ADD I3
00511  0 76500 0  00043         LRS 35
00512  0 20000 0  77761         MPY K2
00513  0 76300 0  00042         LLS 34
00514  0 73400 1  00000         PAX 0,1
00515  0 60000 1  00000  XJA3   STZ 0,1                ADDRESS TO BE SET
00516  2 00001 1  00515         TIX XJA3,1,1
00517  0 53400 4  00721  XJB    LXA I4,4
00520  0 76200 0  00225  XJB1   RTB U3
00521  2 00001 4  00520         TIX XJB1,4,1
00522  0 53400 4  00720  XJC    LXA I3,4
```

```
00523 -0 63400 4 00724  XJD    SXD T301,4
00524  0 76200 0 00225         RTB U3
00525 -0 76000 0 00012         RTT
00526  0 76100 0 00000         NOP
00527  0 70000 0 00725  XJE    CPY T302
00530  0 02000 0 00533         TRA XJF
00531  0 02000 0 00701         TRA XLE
00532  0 00000 0 00144         HTR RCD                NO WORDS IN RECORD
00533  0 53400 4 00721  XJF    LXA I4,4
00534  0 70000 0 00725  XJF1   CPY T302
00535  2 00001 4 00534         TIX XJF1,4,1
00536  0 70000 0 00726  XJG    CPY T303
00537  0 50000 0 77763  XJH    CLA K4
00540  0 40000 0 00722         ADD I7
00541  0 73400 4 00000         PAX 0,4
00542  0 70000 0 00727  XJH1   CPY T304
00543  2 00001 4 00542         TIX XJH1,4,1
00544  0 70000 0 00730  XJI    CPY T305
00545  0 70000 0 00731  XJJ    CPY T306
00546 -0 53400 4 77764  XJK    LXD K5,4               OR TRA XJS
00547 -0 53400 1 77765         LXD K6,1
00550 -0 53400 2 77766         LXD K7,2
00551 -0 50000 0 77767         CAL K8
00552  0 70000 4 00000  XJL    CPY 0,4
00553  0 02000 0 00556         TRA XJM
00554  0 00000 0 00000         PZE
00555  0 02000 0 00573         TRA XJT
00556 -0 76000 0 00001  XJM    PBT
00557  0 02000 0 00562         TRA XJO
00560  1 77777 4 00561  XJN    TXI XJN1,4,-1
00561 -3 00000 4 00570  XJN1   TXL XJS,4,0            DECREMENT TO BE SET
00562  0 76700 0 00001  XJO    ALS 1
00563  2 00001 1 00552  XJP    TIX XJL,1,1
00564 -2 00001 2 00570  XJQ    TNX XJS,2,1
00565  0 53400 1 00723  XJR    LXA I36,1
00566 -0 50000 2 77760         CAL K1,2
00567  0 02000 0 00552         TRA XJL
00570  0 70000 0 00732  XJS    CPY T307
00571  0 02000 0 00570         TRA XJS
00572  0 00000 0 00000         PZE
00573  0 76600 0 00333  XJT    IOD
00574 -0 76000 0 00012         RTT
00575  0 02000 0 00577         TRA XJU
```

```
00576  0 02000 0 00604          TRA XJX
00577 -0 53400 4 00724  XJU     LXD T301,4
00600 -2 00001 4 00603          TNX XJW,4,1
00601  0 76400 0 00205  XJV     BST U3
00602  0 02000 0 00523          TRA XJD
00603  0 00000 0 00522  XJW     HTR XJC                RTT FAILS 3 TIMES. START TO SKIP RECORD
00604  0 50000 0 00730  XJX     CLA T305
00605 -0 10000 0 00522          TNZ XJC
00606  0 50000 0 00725  XJY     CLA T302
00607  0 10000 0 00522          TZE XJC
00610  0 53400 1 77762  XJZ     LXA K3,1
00611 -3 00000 1 00640          TXL XKK,1,0
00612  0 53400 2 77771          LXA K10,2
00613  0 60000 2 00000  XJZ1    STZ 0,2
00614  1 77777 2 00615          TXI XJZ2,2,-1
00615  2 00001 1 00613  XJZ2    TIX XJZ1,1,1
00616  0 53400 2 77771  XKA     LXA K10,2
00617  0 53400 4 00726          LXA T303,4
00620  0 53400 1 77760          LXA K1,1
00621 -0 50000 1 77760  XKB     CAL K1,1
00622 -0 63400 1 00724          SXD T301,1
00623  0 53400 1 00723          LXA I36,1
00624 -0 76000 0 00001  XKC     PBT
00625  0 02000 0 00633          TRA XKG
00626  2 00001 4 00632  XKD     TIX XKF,4,1
00627  0 56000 0 00731  XKE     LDQ T306
00630 -0 60000 2 00000          STQ 0,2
00631  0 02000 0 00640          TRA XKK
00632  1 77777 2 00634  XKF     TXI XKH,2,-1
00633 -2 00001 4 00640  XKG     TNX XKK,4,1
00634  0 76700 0 00001  XKH     ALS 1
00635  2 00001 1 00624  XKI     TIX XKC,1,1
00636 -0 53400 1 00724  XKJ     LXD T301,1
00637  2 00001 1 00621          TIX XKB,1,1
00640  0 53400 1 77761  XKK     LXA K2,1
00641  0 56000 0 00725  XKK1    LDQ T302
00642  0 26000 1 00000  XKK2    FMP 0,1                ADDRESS TO BE SET
00643  0 60100 1 00000  XKK3    STO 0,1                ADDRESS TO BE SET
00644  2 00001 1 00641          TIX XKK1,1,1
00645  0 50000 0 77772  XKL     CLA K11                OR TRA XKS
00646  0 62100 0 00655          STA XKO2
00647  0 62100 0 00656          STA XKO3
00650  0 53400 1 77761  XKM     LXA K2,1
```

```
00651 -0 75400 1 00000  XKN   PXD 0,1
00652 -0 73400 2 00000        PDX 0,2
00653  0 56000 1 00000  XKO   LDQ 0,1                ADDRESS TO BE SET
00654  0 26000 2 00000  XKO1  FMP 0,2                ADDRESS TO BE SET
00655  0 30000 2 00000  XKO2  FAD 0,2                ADDRESS TO BE SET
00656  0 60100 2 00000  XKO3  STO 0,2                ADDRESS TO BE SET
00657  2 00001 2 00653  XKP   TIX XKO,2,1
00660 -2 00001 1 00667  XKQ   TNX XKS,1,1
00661 -0 75400 1 00000  XKR   PXD 0,1
00662  0 77100 0 00022        ARS 18
00663  0 40000 0 00655        ADD XKO2
00664  0 62100 0 00655        STA XKO2
00665  0 62100 0 00656        STA XKO3
00666  0 02000 0 00651        TRA XKN
00667  0 53400 1 77761  XKS   LXA K2,1
00670  0 56000 0 00725        LDQ T302
00671  0 26000 0 00727        FMP T304
00672  0 60100 0 00727        STO T304
00673  0 56000 0 00727  XKT   LDQ T304
00674  0 26000 1 00000  XKT1  FMP 0,1                ADDRESS TO BE SET
00675  0 30000 1 00000  XKT2  FAD 0,1                ADDRESS TO BE SET
00676  0 60100 1 00000  XKT3  STO 0,1                ADDRESS TO BE SET
00677  2 00001 1 00673  XKU   TIX XKT,1,1
00700  0 02000 0 00522        TRA XJC
00701  0 76200 0 00225  XLE   RTB U3
00702  0 07400 4 00146  XLF   TSX WTB,4
00703  0 00000 0 00005        PZE U3
00704  0 77054 0 77323        PZE -START,0,-I36-1
00705  0 50000 0 77777  XLG   CLA K16
00706  0 60100 0 00711        STO XLG1
00707  0 07400 4 00146        TSX WTB,4
00710  0 00000 0 00005        PZE U3
00711  0 00000 0 00000  XLG1  PZE                    TO BE SET
00712  0 02000 0 00144        TRA RCD                ENTER OR-XLS4
                                  SENSE-SETTING WORDS
00713  0 02000 0 00667        TRA XKS
00714  0 50000 0 77772  3XKL  CLA K11
00715  0 02000 0 00570        TRA XJS
00716 -0 53400 4 77764  1XJK  LXD K5,4
00717  0 00000 0 00001  I1    PZE 1
00720  0 00000 0 00003  I3    PZE 3
00721  0 00000 0 00004  I4    PZE 4
00722  0 00000 0 00007  I7    PZE 7
```

```
00723  0 00000 0 00044  I36   PZE 36
00724  0 00000 0 00000  T301                        INDEX STORED IN DECREMENT
00725  0 00000 0 00000  T302                        SQRT W
00726  0 00000 0 00000  T303                        SCALE FACTOR IDENTIFICATION
00727  0 00000 0 00000  T304                        OBS-CALC
00730  0 00000 0 00000  T305                        REJECTION INDICATOR
00731  0 00000 0 00000  T306                        D CALC/D SCALE
00732  0 00000 0 00000  T307                        DISCARDS ARE COPIED HERE
                                THE PROGRAM ASSIGNS THE FOLLOWING STORAGE
                                IMMEDIATELY PRECEEDING INTERSEGMENT STORAGE-
                                    N LOCATIONS FOR THOSE DERIVATIVES USED.
                                    N(N+1)/2 LOCATIONS FOR THE MATRIX.
                                    N LOCATIONS FOR THE VECTOR.
                                    PARAMETER SELECTION WORDS.
                                INTERSEGMENT TEMPORARY STORAGE
                77760  K1    EQU 32752              NUMBER OF PARAMETER SELECTION WORDS
                77761  K2    EQU K1+1               NUMBER OF PARAMETERS TO BE VARIED
                77762  K3    EQU K2+1               NUMBER OF SCALE FACTORS TO BE VARIED
                77763  K4    EQU K3+1               NUMBER OF KINDS OF FORM FACTORS
                77764  K5    EQU K4+1               COMP. DERIV. ADDRESS IN DECREMENT
                77765  K6    EQU K5+1               BIT COUNTER IN DECREMENT
                77766  K7    EQU K6+1               SELECTION WORD COUNTER IN DECREMENT
                77767  K8    EQU K7+1               PARTLY SHIFTED SELECTION WORD
                77770  K9    EQU K8+1               BY-PASS INDICATOR
                77771  K10   EQU K9+1               COMP. INITIAL DERIVATIVE ADDRESS
                77772  K11   EQU K10+1              INITIAL MATRIX ADDRESS +N
                77773  K12   EQU K11+1              INITIAL VECTOR ADDRESS
                77774  K13   EQU K12+1              MODE NUMBER
                77775  K14   EQU K13+1              INITIAL MATRIX ADDRESS
                77776  K15   EQU K14+1              INITIAL SELECTION WORD ADDRESS
                77777  K16   EQU K15+1              -MATRIX ADDRESS,0,-VECTOR ADDRESS
                00000        END 0
```

```
                                    OR-XLS4   MATRIX INVERSION SEGMENT
                  00004  U1     EQU 4                  NUMBER OF BINARY INPUT TAPE
                  00005  U3     EQU 5                  NUMBER OF BINARY OUTPUT TAPE
                  00144  RCD    EQU 100
                  00146  WTB    EQU 102
                  00147  RTB    EQU 103
                  00455         ORG 301
00455  0 02000 0  00461  START  TRA XMA
00456  0 00000 0  00144         HTR RCD                NO ENTRY HERE
00457  0 02000 0  00144         TRA RCD
00460  0 00000 0  00144         HTR RCD                NO ENTRY HERE
00461  0 53400 4  77774  XMA    LXA K13,4
00462  3 00003 4  00504         TXH XMF,4,3
00463  0 50000 0  77761  XMB    CLA K2
00464  0 76700 0  00022         ALS 18
00465  0 62200 0  00471         STD XMC1
00466  0 50000 0  77777         CLA K16
00467  0 62100 0  00471         STA XMC1
00470  0 07400 4  00514  XMC    TSX SMI,4
00471  0 00000 0  00000  XMC1   PZE                    TO BE SET
00472  0 00000 0  00144         HTR RCD                MATRIX IS SINGULAR
00473  0 07400 4  00146  XMD    TSX WTB,4
00474  0 00000 0  00005         PZE U3
00475  0 76720 0  77323         PZE -START,0,-SMI-228
00476  0 50000 0  77777  XME    CLA K16
00477  0 60100 0  00502         STO XME1
00500  0 07400 4  00146         TSX WTB,4
00501  0 00000 0  00005         PZE U3
00502  0 00000 0  00000  XME1   PZE                    TO BE SET
00503  0 02000 0  00144         TRA RCD                ENTER OR-XLS5
00504  0 50000 0  77777  XMF    CLA K16
00505  0 62100 0  00510         STA XMF1
00506  0 07400 4  00147         TSX RTB,4
00507  0 00000 0  00004         PZE U1
00510  0 00000 0  00000  XMF1   PZE                    ADDRESS TO BE SET
00511  0 00000 0  00144         HTR RCD                END OF FILE
00512  0 76400 0  00204         BST U1
00513  0 02000 0  00473         TRA XMD
                  00514  SMI    BSS 228
                                    THE PROGRAM ASSIGNS THE FOLLOWING STORAGE
                                    IMMEDIATELY PRECEEDING INTERSEGMENT STORAGE-
                                        N LOCATIONS USED BY OR SMI
                                        N(N+1)/2 LOCATIONS FOR THE MATRIX.
```

```
                                    N LOCATIONS FOR THE VECTOR.
                                    PARAMETER SELECTION WORDS.
                                INTERSEGMENT TEMPORARY STORAGE
                77760  K1    EQU 32752              NUMBER OF PARAMETER SELECTION WORDS
                77761  K2    EQU K1+1               NUMBER OF PARAMETERS TO BE VARIED
                77762  K3    EQU K2+1               NUMBER OF SCALE FACTORS TO BE VARIED
                77763  K4    EQU K3+1               NUMBER OF KINDS OF FORM FACTORS
                77764  K5    EQU K4+1               COMP. DERIV. ADDRESS IN DECREMENT
                77765  K6    EQU K5+1               BIT COUNTER IN DECREMENT
                77766  K7    EQU K6+1               SELECTION WORD COUNTER IN DECREMENT
                77767  K8    EQU K7+1               PARTLY SHIFTED SELECTION WORD
                77770  K9    EQU K8+1               BY-PASS INDICATOR
                77771  K10   EQU K9+1               COMP. INITIAL DERIVATIVE ADDRESS
                77772  K11   EQU K10+1              INITIAL MATRIX ADDRESS +N
                77773  K12   EQU K11+1              INITIAL VECTOR ADDRESS
                77774  K13   EQU K12+1              MODE NUMBER
                77775  K14   EQU K13+1              INITIAL MATRIX ADDRESS
                77776  K15   EQU K14+1              INITIAL SELECTION WORD ADDRESS
                77777  K16   EQU K15+1              -MATRIX ADDRESS,0,-VECTOR ADDRESS
                                THIS SECTION PRODUCES AN ORIGIN CARD FOR THE SUBROUTINE
                00000         ORG 0
00000   0 00000 0 00000       PZE
00001   0 00000 0 00514       PZE SMI
                00000         END 0
```

```
                                        OR-XLS5   MATRIX-VECTOR MULTIPLICATION SEGMENT
                  00005  U3     EQU 5                  NUMBER OF BINARY OUTPUT TAPE
                  00144  RCD    EQU 100
                  00146  WTB    EQU 102
                  00155  KE     EQU 109
                  00455         ORG 301
00455  0 02000 0 00461  START  TRA XNA
00456  0 00000 0 00144         HTR RCD                NO ENTRY HERE
00457  0 02000 0 00144         TRA RCD
00460  0 00000 0 00144         HTR RCD                NO ENTRY HERE
00461  0 50000 0 77776  XNA    CLA K15
00462  0 62100 0 00475         STA XND1
00463  0 62100 0 00517         STA XNHH2
00464  0 50000 0 77775         CLA K14
00465  0 62100 0 00507         STA XNG
00466  0 62100 0 00534         STA XNL
00467  0 53400 4 77777  XNB    LXA K16,4
00470  0 53400 1 77761         LXA K2,1
00471  0 60000 0 00566  XNC    STZ T501
00472 -0 63400 4 00571         SXD T504,4
00473  0 53400 2 77761         LXA K2,2
00474  0 56000 4 00000  XND    LDQ 0,4
00475  0 26000 2 00000  XND1   FMP 0,2                ADDRESS TO BE SET
00476  0 30000 0 00566         FAD T501
00477  0 60100 0 00566         STO T501
00500 -2 00001 2 00507  XNE    TNX XNG,2,1
00501 -0 63400 2 00502  XNEE   SXD XNEE1,2
00502  3 00000 1 00506  XNEE1  TXH XNFF,1,0           DECREMENT TO BE SET
00503 -0 63400 2 00504  XNF    SXD XNF1,2
00504  2 00000 4 00474  XNF1   TIX XND,4,0            DECREMENT TO BE SET
00505  0 00000 0 00144         HTR RCD
00506  1 77777 4 00474  XNFF   TXI XND,4,-1
00507  0 60100 1 00000  XNG    STO 0,1                ADDRESS TO BE SET
00510 -2 00001 1 00513  XNH    TNX XNHH,1,1
00511 -0 53400 4 00571  XNCC   LXD T504,4
00512  1 77777 4 00471         TXI XNC,4,-1
00513  0 60000 0 00570  XNHH   STZ T503
00514  0 53400 1 77771         LXA K10,1
00515  0 53400 2 77761         LXA K2,2
00516  0 56000 1 00000  XNHH1  LDQ 0,1
00517  0 26000 2 00000  XNHH2  FMP 0,2                ADDRESS TO BE SET
00520  0 30000 0 00570         FAD T503
00521  0 60100 0 00570         STO T503
```

```
00522  1 77777 1 00523        TXI XNHH3,1,-1
00523  2 00001 2 00516  XNHH3 TIX XNHH1,2,1
00524  0 07400 4 00146  XNI   TSX WTB,4
00525  0 00000 0 00005        PZE U3
00526  0 77212 0 77323        PZE -START,0,-I8-1
00527  0 53400 4 00564  XNJ   LXA I3,4
00530  0 76600 0 00225  XNK   WTB U3
00531  0 53400 1 77761        LXA K2,1
00532  0 53400 2 77777        LXA K16,2
00533  0 70000 0 00570        CPY T503
00534  0 70000 1 00000  XNL   CPY 0,1                ADDRESS TO BE SET
00535  0 70000 2 00000        CPY 0,2
00536 -0 63400 1 00537  XNM   SXD XNM1,1
00537  2 00000 2 00541  XNM1  TIX XNN,2,0            DECREMENT TO BE SET
00540  0 00000 0 00144        HTR RCD
00541  2 00001 1 00534  XNN   TIX XNL,1,1
00542  0 76400 0 00205  XNO   BST U3
00543  0 76200 0 00225        RTB U3
00544 -0 76000 0 00012        RTT
00545  0 76100 0 00000        NOP
00546  0 70000 0 00567  XNP   CPY T502
00547  0 02000 0 00546        TRA XNP
00550  0 00000 0 00000        PZE
00551  0 76600 0 00333  XNQ   IOD
00552 -0 76000 0 00012        RTT
00553  0 02000 0 00561        TRA XNT
00554  0 77000 0 00205  XNR   WEF U3
00555  0 53400 4 00565  XNS   LXA I8,4
00556  0 76400 0 00205  XNS1  BST U3
00557  2 00001 4 00556        TIX XNS1,4,1
00560  0 02000 0 00155        TRA KE
00561  0 76400 0 00205  XNT   BST U3
00562  2 00001 4 00530  XNU   TIX XNK,4,1
00563  0 00000 0 00527  XNV   HTR XNJ                RTT FAILS 3 TIMES. START TO TRY AGAIN
00564  0 00000 0 00003  I3    PZE 3
00565  0 00000 0 00010  I8    PZE 8
00566  0 00000 0 00000  T501                         COMPUTED PARAMETER CHANGE, X(I)
00567  0 00000 0 00000  T502                         DISCARDS COPIED HERE
00570  0 00000 0 00000  T503                         CORRECTION TO SUM W(OBS-CALC)**2
00571  0 00000 0 00000  T504                         INITIAL ADDRESS SAVED HERE
                                THE PROGRAM ASSIGNS THE FOLLOWING STORAGE
                                IMMEDIATELY PRECEEDING INTERSEGMENT STORAGE-
                                    N LOCATIONS FOR THE COMPUTED PARAMETER CHANGES
```

```
                    N(N+1)/2 LOCATIONS FOR THE MATRIX.
                    N LOCATIONS FOR THE VECTOR.
                    PARAMETER SELECTION WORDS.
                INTERSEGMENT TEMPORARY STORAGE
77760  K1    EQU 32752          NUMBER OF PARAMETER SELECTION WORDS
77761  K2    EQU K1+1           NUMBER OF PARAMETERS TO BE VARIED
77762  K3    EQU K2+1           NUMBER OF SCALE FACTORS TO BE VARIED
77763  K4    EQU K3+1           NUMBER OF KINDS OF FORM FACTORS
77764  K5    EQU K4+1           COMP. DERIV. ADDRESS IN DECREMENT
77765  K6    EQU K5+1           BIT COUNTER IN DECREMENT
77766  K7    EQU K6+1           SELECTION WORD COUNTER IN DECREMENT
77767  K8    EQU K7+1           PARTLY SHIFTED SELECTION WORD
77770  K9    EQU K8+1           BY-PASS INDICATOR
77771  K10   EQU K9+1           COMP. INITIAL SOLUTION ADDRESS
77772  K11   EQU K10+1          INITIAL MATRIX ADDRESS +N
77773  K12   EQU K11+1          INITIAL VECTOR ADDRESS
77774  K13   EQU K12+1          MODE NUMBER
77775  K14   EQU K13+1          INITIAL MATRIX ADDRESS
77776  K15   EQU K14+1          INITIAL SELECTION WORD ADDRESS
77777  K16   EQU K15+1          -MATRIX ADDRESS,0,-VECTOR ADDRESS
00000        END 0
```

```
                                        OR XLS6   OUTPUT OF MATRIX OR INVERSE
                  00455  START EQU 301                  REFERS TO OR XLS2
                  10406  T55   EQU 4358                 REFERS TO OR XLS2
                  77761  K2    EQU 32753                REFERS TO OR XLS2
                  00125        ORG 85
00125  0 77200 0 00205  MA    REW 5
00126  0 50000 0 01314  MB    CLA N
00127 -0 10000 0 00142        TNZ ME
00130  0 76200 0 00225  MC    RTB 5
00131  0 76200 0 00225        RTB 5
00132  0 07400 4 00343        TSX RTB,4
00133  0 00000 0 00005        PZE 5
00134  0 00000 0 76463        PZE -A
00135  0 00000 0 00000        HTR 0                    END OF FILE
00136  0 50000 0 01676        CLA A-32512+K2
00137  0 60100 0 01314        STO N
00140 -0 10000 0 00142  MD    TNZ ME
00141  0 00000 0 00000        HTR 0                    N IS ZERO
00142  0 76200 0 00225  ME    RTB 5
00143  0 70000 0 01315        CPY A
00144  0 02000 0 00142        TRA ME
00145  0 02000 0 00147        TRA ME1
00146  0 02000 0 00142        TRA ME
00147  0 07400 4 00343  ME1   TSX RTB,4
00150  0 00000 0 00005        PZE 5
00151  0 00000 0 76463        PZE -A
00152  0 00000 0 00000        HTR 0                    END OF FILE. TAPE IS INCOMPLETE.
00153  0 53400 4 00426        LXA I12,4
00154  0 50000 4 11262  ME2   CLA A-START+T55+12,4
00155  0 60100 4 00445        STO TITLE+12,4
00156  2 00001 4 00154        TIX ME2,4,1
00157  0 76200 0 00225        RTB 5
00160  0 76000 0 00165  MF    SWT 5
00161  0 02000 0 00166        TRA MH
00162  0 76200 0 00225  MG    RTB 5
00163  0 76200 0 00225        RTB 5
00164  0 50000 0 00417        CLA C5
00165  0 60100 0 00245        STO MP2
00166  0 07400 4 00343  MH    TSX RTB,4
00167  0 00000 0 00005        PZE 5
```

```
00170  0 00000 0 76463          PZE -A
00171  0 00000 0 00000          HTR 0                    END OF FILE
00172  0 77200 0 00205          REW 5
00173  0 53400 1 01314  MI      LXA N,1
00174 -0 63400 1 00341          SXD MX1,1
00175  0 53400 1 00425          LXA I1,1
00176 -0 63400 1 00274  MJ      SXD MS,1
00177 -0 75400 1 00000          PXD 0,1
00200  0 77100 0 00022          ARS 18
00201  0 60100 0 00445          STO J1
00202  0 50000 0 00424          CLA C10
00203  0 40200 0 00445          SUB J1
00204  0 73400 2 00000          PAX 0,2
00205  0 53400 4 00430  MK      LXA I16,4
00206  0 50000 4 00414  MK1     CLA C2+16,4
00207  0 60100 4 00330          STO MU+18,4
00210  2 00001 4 00206          TIX MK1,4,1
00211  0 53400 4 00427  ML      LXA I13,4
00212  0 50000 0 00445          CLA J1
00213  0 40000 0 00425  ML1     ADD I1
00214  0 60100 4 00463          STO J1+14,4
00215  2 00001 4 00213          TIX ML1,4,1
00216  0 50000 0 00462  MM      CLA J2
00217  0 40200 0 01314          SUB N
00220 -0 12000 0 00234          TMI MO
00221  0 10000 0 00234          TZE MO
00222  0 73400 4 00000  MN      PAX 0,4
00223  0 50000 0 00373          CLA C1
00224  0 60100 4 00330          STO MV,4
00225  0 50000 0 00423          CLA C9
00226  0 60100 4 00265          STO MP1,4
00227  0 50000 0 00413          CLA C2+15
00230  0 60100 4 00327          STO MV-1,4
00231  0 60100 4 00264          STO MP1-1,4
00232  0 53400 4 01314          LXA N,4
00233  0 02000 0 00235          TRA MO1
00234  0 53400 4 00462  MO      LXA J2,4
00235 -0 63400 4 00336  MO1     SXD MW1,4
00236  0 07400 4 00463  MO2     TSX OUT,4
00237  0 00000 0 00236          HTR MO2
```

```
00240  3 27451 0 00431        PTH TITLE,0,12073
00241  3 02066 0 00420        PTH C6,0,1078
00242  1 00001 0 00003        PON 3,0,1
00243  0 07400 4 00463  MP    TSX OUT,4
00244  0 00000 0 00243        HTR MP
00245  3 01757 0 00414  MP2   PTH C3,0,1007
00246 -0 00016 0 00445        FOR J1,0,14
00247 -0 00026 0 00446        FOR J1+1,0,22
00250 -0 00036 0 00447        FOR J1+2,0,30
00251 -0 00046 0 00450        FOR J1+3,0,38
00252 -0 00056 0 00451        FOR J1+4,0,46
00253 -0 00066 0 00452        FOR J1+5,0,54
00254 -0 00076 0 00453        FOR J1+6,0,62
00255 -0 00106 0 00454        FOR J1+7,0,70
00256 -0 00116 0 00455        FOR J1+8,0,78
00257 -0 00126 0 00456        FOR J1+9,0,86
00260 -0 00136 0 00457        FOR J1+10,0,94
00261 -0 00146 0 00460        FOR J1+11,0,102
00262 -0 00156 0 00461        FOR J1+12,0,110
00263 -0 00166 0 00462        FOR J1+13,0,118
00264  1 00060 0 00003        PON 3,0,48
00265  0 07400 4 00463  MP1   TSX OUT,4
00266  0 00000 0 00245        HTR MP2
00267  1 00060 0 00003        PON 3,0,48
00270  0 53400 1 00425  MQ    LXA I1,1
00271 -0 75400 1 00000  MR    PXD 0,1
00272  0 77100 0 00022        ARS 18
00273  0 60100 0 01313        STO I
00274 -3 00000 1 00306  MS    TXL MU,1,0            J1 SET IN DECREMENT
00275  0 50000 0 00462  MT    CLA J2
00276  0 40200 0 01313        SUB I
00277  0 73400 4 00000        PAX 0,4
00300  0 50000 4 00262        CLA MP+15,4
00301  0 60100 4 00325        STO MU+15,4
00302  0 50000 0 00422        CLA C8
00303  0 62100 4 00325        STA MU+15,4
00304  0 50000 0 00421        CLA C7
00305  0 60100 4 00324        STO MU+14,4
00306  0 07400 4 00463  MU    TSX OUT,4
00307  0 00000 0 00306        HTR MU
```

```
                  00310          BSS 16
00330  0 50000 0 01314  MV      CLA N
00331  0 40200 0 01313          SUB I
00332  0 76700 0 00022          ALS 18
00333  0 62200 0 00334          STD MV1
00334  2 00000 2 00335  MV1     TIX MW,2,0              DECREMENT SET AT N-I
00335  1 00001 1 00336  MW      TXI MW1,1,1
00336 -3 00000 1 00271  MW1     TXL MR,1,0              DECREMENT SET AT J2
00337  0 53400 1 00445  MX      LXA J1,1
00340  1 00016 1 00341          TXI MX1,1,14
00341 -3 00000 1 00176  MX1     TXL MJ,1,0              DECREMENT SET AT N
00342  0 00000 0 00000          HTR 0                   END OF PROGRAM
                                    SUBROUTINE TO READ RECORD FROM TAPE
00343  0 50000 4 00001  RTB     CLA 1,4
00344  0 40000 0 00371          ADD RTB7
00345  0 60100 0 00354          STO RTB3
00346  0 50000 4 00001          CLA 1,4
00347  0 40000 0 00372          ADD RTB8
00350  0 60100 0 00366          STO RTB6
00351 -0 53400 1 00364  RTB1    LXD RTB5,1
00352  0 50000 4 00002  RTB2    CLA 2,4
00353  0 73400 2 00000          PAX 0,2
00354  0 76200 0 00220  RTB3    RTB 0                   TO BE SET
00355 -0 76000 0 00012          RTT
00356  0 76100 0 00000          NOP
00357  0 70000 2 00000  RTB4    CPY 0,2
00360  1 77777 2 00357          TXI RTB4,2,-1
00361  0 02000 4 00003          TRA 3,4
00362  0 76600 0 00333          IOD
00363 -0 76000 0 00012          RTT
00364  1 00003 0 00366  RTB5    TXI RTB6,0,3
00365  0 02000 4 00004          TRA 4,4
00366  0 76400 0 00200  RTB6    BST 0                   TO BE SET
00367  2 00001 1 00352          TIX RTB2,1,1
00370  0 00000 0 00351          HTR RTB1                RTT FAILS 3 TIMES. START TO TRY AGAIN.
00371  0 76200 0 00220  RTB7    RTB 0                   CONSTANT
00372  0 76400 0 00200  RTB8    BST 0                   CONSTANT
00373  0 02000 0 00330  C1      TRA MV
00374 -0 00006 0 01313  C2      FOR I,0,6
00375 -2 05710 2 01314          SIX A-1,2,3016
```

```
00376 -2 05720 2 01315          SIX A,2,3024
00377 -2 05730 2 01316          SIX A+1,2,3032
00400 -2 05740 2 01317          SIX A+2,2,3040
00401 -2 05750 2 01320          SIX A+3,2,3048
00402 -2 05760 2 01321          SIX A+4,2,3056
00403 -2 05770 2 01322          SIX A+5,2,3064
00404 -2 06000 2 01323          SIX A+6,2,3072
00405 -2 06010 2 01324          SIX A+7,2,3080
00406 -2 06020 2 01325          SIX A+8,2,3088
00407 -2 06030 2 01326          SIX A+9,2,3096
00410 -2 06040 2 01327          SIX A+10,2,3104
00411 -2 06050 2 01330          SIX A+11,2,3112
00412 -2 06060 2 01331          SIX A+12,2,3120
00413  1 00060 0 00003          PON 3,0,48
00414  442163513167      C3     BCD 1MATRIX
00415  314565255162      C4     BCD 2INVERSE
00416  256060606060
00417  3 03735 0 00415   C5     PTH C4,0,2013
00420  606060606060      C6     BCD 1
00421  3 01757 0 00420   C7     PTH C6,0,1007
00422  0 00000 0 01313   C8     PZE I
00423  0 02000 0 00265   C9     TRA MP1
00424  2 00000 0 00000   C10    PTW                    LARGE POSITIVE INTEGER
00425  0 00000 0 00001   I1     PZE 1
00426  0 00000 0 00014   I12    PZE 12
00427  0 00000 0 00015   I13    PZE 13
00430  0 00000 0 00020   I16    PZE 16
                 00431   TITLE BSS 12
                 00445   J1     BSS 13                 FIRST COLUMN IN SECTION
00462  0 00000 0 00000   J2                            LAST COLUMN IN SECTION
                 00463   OUT    BSS 408
01313  0 00000 0 00000   I                             CURRENT ROW NUMBER
01314  0 00000 0 00000   N                             ORDER OF MATRIX
01315  0 00000 0 00000   A                             START OF STORAGE AREA
                                   ORIGIN CARD FOR OUT
                 00000          ORG 0
00000  0 00000 0 00000          PZE
00001  0 00000 0 00463          PZE OUT
                 00125          END MA
```

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by W. R. Busing and H. A. Levy

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A CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM FOR THE IBM 704

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A CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM FOR THE IBM 704

by

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Oak Ridge, Tennessee

December, 1959

IDENTIFICATION

OR XFE

DATE ISSUED

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GENERAL DESCRIPTION

Given the unit cell parameters of a crystal together with the atomic coordinates and/or the anisotropic temperature factor coefficients, this program will compute various functions of these parameters such as the distance between two atoms, an angle defined by three atoms, the principal axes of the anisotropic temperature factor, etc. Furthermore, if the errors of the input parameters are available to the program in the form of a variance-covariance matrix obtained, for example, from the inverse matrix of a least squares refinement, then the program will also compute the standard errors of the various functions with and without the contribution of the cell parameter errors. This program may be used independently, reading all input data from cards, or it may be used in conjunction with the least squares refinement program OR XLS1-6, in which case much of the input is taken from the binary output tape of a cycle of least squares.

The various types of functions which can be evaluated are defined by subroutines, fifteen of which are included in the present program. The detailed specification of each function or group of functions to be computed is made by means of an instruction card which will be described below. If functions are desired other than those already included the user need only write a Fortran II subroutine for the function, compile it, and add it to the deck. To facilitate such programming several subroutines for the manipulation of matrices and vectors are included in the program, and descriptions of these will be given below together with detailed specifications for writing subroutines for new functions.

MACHINE REQUIREMENTS

Minimum 704 with

1. 8192 word core storage or more.*
2. 3 on-line tape units.
3. CAD instruction.
4. Off-line tape printer.

*See "Operating Procedure" and "Specifications for Subroutines to Compute New Types of Functions" for special procedures to be followed when an 8192 word machine is used.

MATHEMATICAL METHOD

The functions which the program computes are of the form

$$f = f(p_1, p_2, p_3 \ldots\ldots a_1, a_2 \ldots\ldots a_6)$$

where the p's are the atomic parameters and the a's are the unit cell parameters. Each kind of f is computed by a special subroutine for this purpose, and the mathematical expressions are best obtained from the Fortran language listings of these subroutines designated FUN1, FUN2, etc.

The standard error of f is given by

$$e = (e'^2 + e''^2)^{1/2}$$

where

$$e'^2 = \sum_{j=i}^{n} \sum_{i=1}^{n} (2 - \delta_{ij}) \left(\frac{\partial f}{\partial p_i}\right)\left(\frac{\partial f}{\partial p_j}\right) V_{ij}$$

and

$$e''^2 = \sum_{j=i}^{6} \sum_{i=1}^{6} (2 - \delta_{ij}) \left(\frac{\partial f}{\partial a_i}\right)\left(\frac{\partial f}{\partial a_j}\right) U_{ij}.$$

Here V_{ij} is an element of the variance-covariance matrix which describes the errors of the atomic parameters, and U_{ij} is an element of a similar matrix for the unit cell parameters.

When errors are to be computed the user has the option of obtaining $\underset{\sim}{V}$ from the binary output tape of OR XLS. In this case the program stores

$$V_{ij} = \left[\sum w(\text{OBS} - \text{CALC})^2/(m-n) \right] b_{ij}$$

where b_{ij} is an element of the inverse matrix of the normal equations, and the constant in brackets is the sum of the weighted residuals squared divided by the number of degrees of freedom. The other option available to the user is to read V_{ij} directly from cards.

The unit cell errors may be put in in two ways. If no covariances are known then the user may supply only the six standard errors $\sigma(a_i)$. The program then sets

$$U_{ii} = \sigma^2(a_i)$$
$$U_{ij} = 0, \; i \neq j .$$

Alternatively the 21 independent values of U_{ij} $(i \leq j)$ can be read from cards.

The necessary derivatives are computed numerically by adding an increment Δp_i to p_i and re-entering the subroutine for f. The derivative is then

$$\frac{\partial f}{\partial p_i} \approx \frac{f(p_1,p_2\ldots p_i + \Delta p_i \ldots a_1 \ldots) - f(p_1,p_2\ldots p_i \ldots a_1 \ldots)}{\Delta p_i} .$$

The increment used is $\Delta p_i = (0.01)V_{ii}^{1/2}$. The derivatives with respect to the cell parameters are obtained similarly.

The program is arranged so that it computes derivatives only with respect to the parameters actually involved in f. The information as to which these are is provided by the subroutines PRE1, PRE2, etc., which are supplied for each type of function. Derivative computations are also omitted with respect to fixed parameters which are not represented in the variance-covariance matrix (e.g., the coordinates of atoms in special positions).

Note that for the derivative computation to be correct all symmetry transformations must be made after Δp_i has been added to p_i. Similarly all constraints on the parameters must be set after incrementing. (See the section entitled "Constraints on the Parameters".) In other words, the function f is always computed directly from the fundamental parameters, the errors of which are described by the matrices $\underset{\sim}{V}$ and $\underset{\sim}{U}$.

The output of the program includes a description of the function, the value, f, of the function, the standard error, e, of the function, and e', the standard error not including the effect of unit cell errors.

CONSTRAINTS ON THE PARAMETERS

In order to insure that this program correctly computes the errors of various functions it is necessary for the user to consider whether the symmetry of the crystal introduces constraints either on the cell parameters, A, or on the atomic parameters, P. A simple case occurs when the symmetry forces a parameter to have a fixed value, and this situation is correctly handled by specifying that the error of this parameter is zero. A more complicated procedure is required when the symmetry imposes a relationship between two or more parameters. In this case one of the interrelated parameters is chosen as independent and a Fortran II subroutine is written to set the values of the dependent parameters in terms of it. The main program will enter this

subroutine immediately before each entry to the function computing subroutine so that the derivatives needed for the error calculation are correctly computed. In the input data the errors associated with the dependent parameters should be set to zero. In the case of atomic parameters from a least squares refinement this is probably automatic since the dependent parameters would not have been varied.

Specifications for Fortran II Subroutines

1. Name the subroutine SETA or SETP.
2. The subroutine has no arguments.
3. Use the standard COMMON and DIMENSION statements such as are used in SEG2 of OR XFE.
4. Write theprograms to set A or P for the dependent variables in terms of the independent variables.
5. Compile with Fortran II and insert just before the transfer card of Segment 2 (see Operating Procedure, page 13). This subroutine will automatically supercede a dummy subroutine of the same name which is part of the program deck.

Example 1

For a hexagonal crystal we have $\cos \gamma = -0.5$ and $a = b$. Choosing a as the independent variable we write the subroutine:

```
C     EXAMPLE 1
      SUBROUTINE SETA
      COMMON (Fill in)
      DIMENSION (Fill in)
      DIMENSION (Fill in)
      A(2) = A(1)
      RETURN
      END (0, 1, 0, 0, 0)
```

The cell parameter errors associated with b and with $\cos \alpha$, $\cos \beta$, and $\cos \gamma$ are put in as zero. The parameter b (i.e. A(2)) which is read in is irrelevant.

Example 2

Let us assume that there are no restrictions on the atomic parameters of atom 1 but atoms 2 and 3 have $y = x$, $\beta_{22} = \beta_{11}$, and $\beta_{23} = -\beta_{13}$. Let us take x, β_{11}, and β_{13} as independent. The subroutine may then be written as follows:

```
C     EXAMPLE 2
      SUBROUTINE SETP
      COMMON (Fill in)
      DIMENSION (Fill in)
      DIMENSION (Fill in)
      DO 1 I = 2, 3
      J = IC(7) * (I-1) + IC(8)
      K = IC(9) * (I-1) + IC(10)
      P (J+1) = P(J)                    (Sets y)
      P (K+1) = P(K)                    (Sets β22)
1     P (K+5) = -P(K+4)                 (Sets β23)
      RETURN
      END (0, 1, 0, 0, 0)
```

This example makes use of the parameter arrangement integers IC(7), IC(8), IC(9), and IC(10) to compute the parameter locations. (See "Atomic Parameters", page 15.) The user may prefer to compute these locations in advance.

SPECIFICATIONS FOR SUBROUTINES TO COMPUTE NEW TYPES OF FUNCTIONS

To program a new type of function the user selects a function designation integer, i, where $1 \leq i \leq 20$. (Function designations 1-15 have already been assigned in the program as written, but these may be redefined if desired.) The user then writes four Fortran II subroutines named HEDi, PREi, FUNi, and OUTi. These are compiled and added to the binary deck before the transfer card of Segment 2. They will automatically supercede dummy subroutines with the same names which are already in the program.*

The programmer should refer to the symbolic listing of functions 1-15 for examples of these routines.

HEDi

The user may omit this subroutine if desired. Its purpose is to put out an overall heading which defines the type of function. It is entered each time the function designation IN(1) is changed.

*When an 8192 word maechine is used the user should check the section "Binary Cards Supplied" to be sure that the memory capacity is not exceeded. Subroutines for functions 1-15 may be omitted entirely if necessary.

1. The subroutine has no arguments.
2. No COMMON or DIMENSION statements are needed.
3. Put out the heading on tape 3.
4. The first Hollerith character should be zero to cause double spacing.
5. More than one line may be put out if desired.

PREi

This subroutine need be included only if standard errors are to be computed. Its purpose is to instruct the program as to which parameters are involved in the function to be computed. The program thus avoids computing unnecessary derivatives.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout Segment 2.
3. Enter the subroutines SETKX and/or SETKB once for each atom involved in the function. See page 9 for more details.

FUNi

The purpose of this subroutine is to compute the desired function given the various input data found in common storage.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout Segment 2.
3. The significance of the instruction integers IN(K) except for IN(1) is at the discretion of the programmer.
4. The necessary atomic coordinates or temperature factor coefficients are called for by means of subroutines ATOM or BETA.
5. If the metric tensors AA or BB are to be used the subroutines STOAA and/or STOBB must be entered.
6. See the section on arithmetic subroutines for their usage.
7. Store the function at FX in common and return.

OUTi

The purpose of this subroutine is to put out the detailed description of the individual function computed. Its inclusion is optional but certainly desirable.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout Segment 2.

3. The description which probably includes the relevant instruction integers, IN, is put out on tape 3.
4. The first character of the first line of this description should be a Hollerith + to suppress spacing.
5. The description should not extend past column 49 or it will print over the computed value of the function.
6. More than one line may be put out if desired.

ARITHMETIC SUBPROGRAMS AVAILABLE FOR PROGRAMMING NEW FUNCTIONS

1. CALL SETKX (IN(K))

Instructs the program to calculate derivatives with respect to the coordinates of the atom designated in IN(K). This subroutine is used by the PREliminary subroutines.

2. CALL SETKB (IN(K))

Instructs the program to calculate derivatives with respect to the anisotropic temperature factor coefficients of the atom designated in IN(K). This subroutine is used by the PREliminary subroutines.

3. CALL STOAA

Stores the 3 x 3 metric tensor $\underset{\sim}{g}$ (where $g_{ij} = \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j$) at AA in common storage.

4. CALL STOBB

Stores the 3 x 3 reciprocal metric tensor $\underset{\sim}{g}^{-1}$ (where $(g^{-1})_{ij} = \underset{\sim}{b}_i \cdot \underset{\sim}{b}_j$) at BB in common storage.

5. CALL ATOM (IN(K),Z)

DIMENSION Z(3)

Stores at Z the coordinates of the atom specified by the instruction integers IN(K) and IN(K+1). These coordinates refer to the triclinic axes. They have been transformed according to the symmetry specified.

6. CALL BETA (IN(K),Z)

DIMENSION Z(3,3)

Stores at Z the 3 x 3 matrix of the temperature factor coefficients of the atom specified by instruction integers IN(K) and IN(K+1). The matrix has been transformed according to the symmetry specified.

7. CALL MM (X, Y, Z)

DIMENSION X(3,3), Y(3,3), Z(3,3)

Performs the matrix multiplication $\underset{\sim}{X}\underset{\sim}{Y} = \underset{\sim}{Z}$. The location of $\underset{\sim}{Z}$ must be different from $\underset{\sim}{X}$ and $\underset{\sim}{Y}$.

8. CALL MV (X, Y, Z)

DIMENSION X(3,3), Y(3), Z(3)

Performs the matrix-vector multiplication $\underset{\sim}{X}\underset{\sim}{Y} = \underset{\sim}{Z}$. The location of $\underset{\sim}{Z}$ must be different from $\underset{\sim}{Y}$.

9. CALL VM (X, Y, Z)

DIMENSION X(3), Y(3,3), Z(3)

Performs the vector-matrix multiplication $\underset{\sim}{X}^T\underset{\sim}{Y} = \underset{\sim}{Z}^T$. The locations of $\underset{\sim}{Z}$ must be different from $\underset{\sim}{X}$.

10. Function VV(X, Y)

DIMENSION X(3), Y(3)

Performs the vector-vector multiplication $\underset{\sim}{X}^T\underset{\sim}{Y} = Z$ (a scalar).

11. Function VMV (W, X, Y)

DIMENSION W(3),X(3,3), Y(3)

Performs the vector-matrix-vector multiplication $\underset{\sim}{W}^T\underset{\sim}{X}\underset{\sim}{Y} = Z$ (a scalar).

12. CALL DIFV (X, Y, Z)

DIMENSION X(3), Y(3), Z(3)

Performs the vector subtraction $\underset{\sim}{X} - \underset{\sim}{Y} = \underset{\sim}{Z}$. $\underset{\sim}{Z}$ may have the same location as $\underset{\sim}{X}$ or $\underset{\sim}{Y}$.

13. CALL SUMV (X, Y, Z)

DIMENSION X(3), Y(3), Z(3)

Performs the vector summation $\underset{\sim}{X} + \underset{\sim}{Y} = \underset{\sim}{Z}$. $\underset{\sim}{Z}$ may have the same location as $\underset{\sim}{X}$ or $\underset{\sim}{Y}$.

14. Function COSVV (X,Y)

DIMENSION X(3), Y(3)

Computes the cosine of the angle defined by vectors $\underset{\sim}{X}$ and $\underset{\sim}{Y}$. These vectors are assumed to refer to the triclinic coordinate system, and it is also assumed that the metric tensor has been stored at AA in common storage.

15. Function ARCCOS (X)

Computes θ, the arc cos of X in degrees. $0 \leq \theta < 180$.

16. CALL NORM (X, Y, Z)

DIMENSION X(3), Y(3), Z(3)

Stores at $\underset{\sim}{Z}$ a vector perpendicular to both $\underset{\sim}{X}$ and $\underset{\sim}{Y}$. The sense of $\underset{\sim}{Z}$ is that of the vector product, $\underset{\sim}{Z} = k\ \underset{\sim}{X} \times \underset{\sim}{Y}$, but its length is arbitrary. All vectors are referred to the triclinic coordinate system, and it is assumed that the reciprocal metric tensor has been stored at BB in common storage.

17. CALL AXES (U, V, X)

DIMENSION U(3), V(3), X(3,3)

Stores three mutually perpendicular vectors of arbitrary length at X(I,1), X(I,2), and X(I,3). X(I,1) = U(I). X(I,2) is normal to $\underset{\sim}{U}$ and $\underset{\sim}{V}$, i.e., in the direction of $\underset{\sim}{U} \times \underset{\sim}{V}$. X(I,3) is normal to X(I,1) and X(I,2) so as to yield a right-handed coordinate system. All these vectors are referred to the triclinic coordinate system, and it is assumed that the reciprocal metric tensor has been stored at BB in common storage.

18. CALL EIGVAL (W,Y)

DIMENSION W(3,3), Y(3)

Stores the three eigenvalues Y of the matrix $\underset{\sim}{W}$.

19. CALL EIGVEC (W,Y,Z)

DIMENSION W(3,3), Z(3)

Given an eigenvalue Y of the matrix $\underset{\sim}{W}$, this subroutine stores the eigenvector $\underset{\sim}{Z}$.

20. Function TRACE (X)

DIMENSION X(3,3)

Computes the trace of the matrix $\underset{\sim}{X}$.

ATOM DESIGNATION AND SYMMETRY TRANSFORMATIONS

In the course of preparing an instruction card to specify a function to be computed it will be necessary to define the one or more atoms involved in this function. This is done by means of an atom designation consisting of the two integers $\underline{a}$ and 100 $\underline{c}$ + $\underline{s}$. Here $\underline{a}$ = 1, 2, 3, ... is the number of the atom in the parameter list, $\underline{s}$ = 0, 1, 2, ... is the number of the symmetry transformation to be applied, and $\underline{c}$ = 0, 1, ... 7 defines the unit cell translations as described below.

The program obtains the coordinates of an atom in the following way.

1. The integer a is used to compute the location of the coordinates in the parameter list and x, y, z are picked up. If a = 0 the program sets x = y = z = 0.

2. These coordinates are then transformed to x', y', z' according to the symmetry information punched on symmetry card s. If s = 0 no transformation is made.

3. The cell translations are then made according to the following table:

c	z"	y"	x"
0	z'	y'	x'
1	z'	y'	x' - 1
2	z'	y' - 1	x'
3	z'	y' - 1	x' - 1
4	z' - 1	y'	x'
5	z' - 1	y'	x' - 1
6	z' - 1	y' - 1	x'
7	z' - 1	y' - 1	x' - 1

(As a memory aid, note that the 1's in this table correspond to the binary representation of c.)

For example, atom (3,208) is atom 3 in the parameter list transformed to symmetry position 8 of cell 2, while atom (5,0) is atom 5 just as it appears in the list of parameters. In the subsequent section we will use the term "molecule" in a non-rigorous way, referring to atom 3 in molecule 208 or atom 5 in the basic molecule (molecule 0).

Note that transformations such as x' = -x and x' = 1-x are not equivalent for purposes of this program.

The program obtains the matrix of the anisotropic temperature factor coefficients of an atom in a similar way except that the elements of this matrix are transformed as the corresponding products of the coordinates. This procedure is valid for an atom in either a special or general position provided that the symmetry card s is written for a general position. (See H. A. Levy, Acta Cryst. (1956). 9,679). The translational part of the symmetry transformation is irrelevant in this case as is the cell translation c. Setting a at zero causes a null matrix to be generated.

OPERATING PROCEDURE

Card deck

If control card (6.b. below) will specify that .....

....no variance-covariance matrix is to be used.	....variance-covariance matrix has been taken from binary output tape of OR XLS.	....variance-covariance matrix has been read from cards.
1. ---	1. Segment 1A (red)	1. Segment 1B (orange)
2. ---	2. ---	2. Data consisting of: a) Variance-covariance matrix.

3. Segment 2 main deck.

   a. Basic program (yellow)
   * b. Functions 1-6 (green)
   * c. Functions 7-11 (blue)
   * d. Functions 12-15 (brown)

   *With 8192 core memory only one of these decks may be used at one time.

4. Any Fortran II subprograms added by user.
5. Segment 2 transfer card. (red stripe)
6. Data consisting of:
   a) Title card.
   b) Control card.
   c) Atomic parameters if called for by control card. Otherwise they are read from binary output tape from OR XLS.
   d) Parameter selection cards if matrix is read from cards and if called for by control card.
   e) Cell parameters.
   f) Cell parameter errors if called for by control card.
   g) Symmetry cards if called for by control card.
   h) Instruction cards.
7. Three blank cards.

Operating instructions

1. Mount a blank tape on unit 3 for BCD output. It will not be rewound by the program before using.
2. If the binary output tape from OR XLS is to be used mount it on unit 5. File protect on if desired.
3. If errors are to be computed mount a blank on unit 6.
4. Clear and load cards. Stops with 77777_8 in storage register.
5. List tape 3, program control, automatic overflow.
6. Hold tape 5 if desired.

DETAILS OF DATA INPUT

All data cards with the exception of the parameter selection cards are read by the Fortran READ subroutines. In the following description the FORMAT statement will be given as an aid to data preparation.

Variance-covariance matrix, PM, for structure parameters

The user has the option of omitting this matrix if errors based on it are not to be computed. When it is to be used it may be read from the binary output tape of OR XLS or from cards prepared as follows:

First card. FORMAT (I9, E9.4)

Columns

1-9 N, the order of the matrix.

10-18 A scale factor by which the matrix will be multiplied. This could be unity or $\Sigma w(F_o-F_c)^2/(m-n)$, for example.

Subsequent cards. FORMAT (8E9.4)

The N(N+1)/2 unique elements of the matrix PM punched eight per card in the order PM(1,1), PM(1,2) .....PM(1,N), PM(2,2), PM(2,3) ....PM(2,N), PM(3,3) .....PM(N,N). The parameters with which this matrix is associated are defined by the parameter selection cards (see below).

Title

FORMAT (72H)

Columns

1 Blank.

2-72 Any desired Hollerith information. This will be printed unchanged on the output.

Control card integers, IC

Ten integers which control the program are read from this card. FORMAT (10I3).

Columns

1-3 IC(1), variance-covariance matrix and parameter selection information will
(0) not be used.
(1) be read from binary output tape of OR XLS.
(2) be read from cards.

4-6 IC(2), number of structure parameters to be read from cards (see below). If IC(2) = 0 these parameters will be read from binary output tape of OR XLS.

7-9 IC(3), cell parameter errors are
(0) not to be used.
(1) to be read in the form of standard errors.
(2) to be read in the form of a variance-covariance matrix.

Control card, cont'd.

Columns

10-12 IC(4), the number of symmetry cards to be read. $0 \leq IC(4) \leq 48$.

13-15 IC(5), the order of the variance-covariance matrix, PM, if it was read from cards (i.e., if IC(1) = 2). Otherwise this control integer is supplied automatically by the program. $1 \leq IC(5) \leq 251$.

16-18 IC(6), the number of parameter-selection cards to be read if matrix was read from cards (i.e., if IC(1) = 2). Otherwise this field is irrelevant. $IC(6) \leq 20$.

The following parameter arrangement integers must be supplied if the structure parameters are read from cards. They are supplied atuomatically by the program if the parameters are read from the binary output tape of OR XLS.

19-21 IC(7), the period of the position parameters in the parameter list. If no position parameters are included in the list then IC(7) and IC(8) are irrelevant.

22-24 IC(8), the position of the first x coordinate in the parameter list.

25-27 IC(9), the period of the temperature factor coefficients in the parameter list. If no temperature factor coefficients are included in the list, then IC(9) and IC(10) are irrelevant.

28-30 IC(10), the position of the first temperature factor coefficient in the parameter list.

Atomic parameters, P

These will be read from the binary output tape of OR XLS if IC(2) = 0. Otherwise IC(2) parameters must be punched eight per card, FORMAT (8E9.4). The arrangement of these parameters is subject to the following restrictions:

a) For each atom the position parameters x, y, z must be in sequence.

b) Position parameters for successive atoms must appear periodically in the order of the atom designation.

c) If anisotropic temperature factor coefficients are included they must be in the sequence β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}, for each atom.

d) Temperature factor coefficients of successive atoms must appear periodically in the order of the atom designation.

Thus the position parameters of atom I start with P(J) where J = IC(7)*(I-1) + IC(8) and the temperature factor coefficients of atom I start with P(K) where K = IC(9)*(I-1) + IC(10).

Parameter selection cards

The purpose of these cards is to identify those parameters which are associated with elements of the variance-covariance matrix. They are exactly the same as the parameter selection cards used with OR XLS.

These cards are not to be supplied unless the control card integer IC(1) specified that the variance-covariance matrix and parameter selection information is to be read from cards. Furthermore, if the variance-covariance matrix of order N corresponds to the first N parameters read, then it is permissible to set IC(6) = 0 and to omit the parameter selection cards.

Each column of a parameter selection card corresponds to one parameter. The first card is associated with parameters 1 to 72, the second with parameters 73 to 144, etc. If a parameter is represented in the matrix a one is punched in the corresponding column, otherwise a zero or a blank is punched. (Actually, all rows but the 1 row are ignored by the program.) The total number of one punches must be equal to N, the order of the matrix. The first parameter in the list for which a one punch is found is assumed to correspond to the first row and column of the matrix, the second with the second, etc.

Cell parameters, A

These six direct unit cell parameters must always be supplied.

FORMAT (6E9.4)

Columns

1-9	A(1) = a
10-18	A(2) = b
19-27	A(3) = c
28-36	A(4) = cos α
37-45	A(5) = cos β
46-54	A(6) = cos γ

Cell parameter errors, AM

The the effect of cell parameter errors is to be considered they must be supplied in one of two forms as specified by the control card integer IC(3).

a) Standard error form, (IC(3) = 1). If this input is used the covariances between the cell parameters are assumed to be zero.

FORMAT (6E9.4)

Columns

1-9	σ(a)
10-18	σ(b)
19-27	σ(c)
28-36	σ(cos α)
37-45	σ(cos β)
47-54	σ(cos γ)

b) Variance-covariance matrix form, (IC(3) = 2). If information on the covariances between cell parameters is available, then the 21 unique elements of this 6 x 6 matrix may be read from three cards.

FORMAT (8E9.4)

Card 1: AM(a,a), AM(a,b) ..... AM(a, cos γ), AM(b,b), AM(b,c).

Card 2: AM(b, cos α) .... AM(b, cos γ), AM(c,c) ..... AM(cos α, cos α).

Card 3: AM(cos α, cos β) ..... AM(cos γ, cos γ).

CAUTION: If symmetry gives rise to constraints on the cell parameters the errors will not be correctly computed unless the instructions in the section "Constraints on the parameters" are followed.

Symmetry cards

The number of symmetry cards to be read is given by IC(4) on the control card. There must be a card for each symmetry transformation which will be called for by an instruction card (see the section on "Specification of an atom"). If the functions to be computed require no symmetry transformations then no symmetry cards need be supplied.

The form of a symmetry card is essentially the same as those for OR XLS2.

FORMAT (E11.8, 4H E11.8, 4H E11.8, 4H)

Columns

1-15 The expression for the transformed coordinate x' as follows:

1-11 Floating point translational part of x' or blank.

12 Hollerith -, +, or blank. The sign associated with the symbol in column 13. Blank and + are equivalent.

13 Hollerith X, Y, Z, or blank.

14 Hollerith -, +, or blank. The sign associated with the symbol in column 15. Blank and + are equivalent.

15 Hollerith X, Y, Z, or blank. Note that columns 12 and 13 are exactly equivalent to 14 and 15. Thus the transformation x' = 1/2-x may be punched

1 ... 11	12	13	14	15
.5	-	X		

or

1 ... 11	12	13	14	15
.5			-	X

.

Note that the expression x' = 2x must be treated as x' = x + x.

16-30 The expression for the transformed coordinate y' as follows:

16-26 The floating point translational part of y' or blank.

27-30 Hollerith sign, symbol, sign, symbol as described above.

31-45 The expression for the transformed coordinate z' as follows:

31-41 Floating point translational part of z' or blank.

42-45 Hollerith sign, symbol, sign, symbol as described above.

CAUTION: Note that transformations such as x' = 1-x and x' = -x are not equivalent in this application.

DETAILS OF INSTRUCTION INPUT

Each function to be computed by the program is specified by a sequence of integers, IN, which are read from one or more instruction cards. The first integer in this sequence, IN(1), defines the type of function to be computed, and the interpretation of the remaining instruction integers will in general be different for different types of functions. Details of the instruction integers for each type of function are given below.

Each instruction card is read with FORMAT (24I3). Of the 24 integers on this card only the first 23 are considered to be part of the instruction, IN. Usually one card will suffice to specify a function, but if a function requires more than 23 integers to define it then up to ten cards may be used with 23 integers on each card. Punching a one (or any non-zero integer) in field 24 of an instruction card indicates that the instruction is continued on the next card.

Function 1

One interatomic distance.

Columns		
1-3	1	
4-6	a_1	atom designation 1.
7-9	$100c_1 + s_1$	
10-12	a_2	atom designation 2.
13-15	$100c_2 + s_2$	

Function 101

All distances (less than d(max)) between atoms in two molecules.

Columns	
1-3	101
4-6	a(max), the number of atoms in the parameter list.
7-9	$100c_1 + s_1$, molecule designation 1.
10-12	---
13-15	$100c_2 + s_2$, molecule designation 2. (This may be the same as 1.)
16-18	The integer 10d(max). If this is left blank then d(max) = 4.0A.

Function 201

All distances (less than d(max)) between atoms in the basic molecule and all molecules (i.e., all combinations of c and s). Note that this does not necessarily compute all distances in the crystal which are less than d(max).

Columns

1-3	201
4-6	a(max), the number of atoms in the parameter list.
7-15	---
16-18	The integer 10d(max). If this is left blank then d(max) = 4.0A.

Function 2

Angle defined by three atoms.

Columns

1-3	2
4-9	Atom designation 1.
10-15	Atom designation 2 (vertex).
16-21	Atom designation 3.

Function 3

Angle between normals to planes each defined by three atoms. The direction of the normals is that of $(\vec{1,2})x(\vec{1,3})$ and $(\vec{4,5})x(\vec{4,6})$ where $\vec{1,2}$ is the vector defined by atom designations 1 and 2, etc.

Columns

1-3	3	
4-9	Atom designation 1	Plane 1
10-15	Atom designation 2	
16-21	Atom designation 3	
22-27	Atom designation 4	Plane 2
28-33	Atom designation 5	
34-39	Atom designation 6	

Function 4

Difference between two interatomic distances.

Columns

1-3	4	
4-9	Atom designation 1	Distance 1
10-15	Atom designation 2	
16-21	Atom designation 3	Distance 2
22-27	Atom designation 4	

Function 5

Difference between two angles each defined by three atoms.

Columns

1-3	5	
4-9	Atom designation 1	Angle 1
10-15	Atom designation 2 (vertex)	
16-21	Atom designation 3	
22-27	Atom designation 4	Angle 2
28-33	Atom designation 5 (vertex)	
34-39	Atom designation 6	

Function 6

The sum of several angles each defined by three atoms.

Columns

1-3	6	
4-6	n, the number of angles to be summed.	
7-12	Atom designation 1	Angle 1
13-18	Atom designation 2 (vertex)	
19-24	Atom designation 3	
25-30	Atom designation 4	Angle 2
31-36	Atom designation 5 (vertex)	
37-42	Atom designation 6	
	etc.	

Function 7

The RMS component of thermal displacement of one atom along principal axis r.

Columns

1-3	7
4-9	Atom designation
10-12	r (= 1, 2, or 3)

Function 107

Same as Function 7 computed for each of the three values of r.

Columns

1-3	107
4-9	Atom designation

Function 207

Same as Function 7 computed for each atom of a given molecule, each with the three values of r.

Columns

1-3	207
4-6	a(max), the number of atoms in the parameter list.
7-9	Molecule designation

Function 8

Angle between principal axis r of atom 1 and a vector defined by atoms 2 and 3.

Columns

1-3	8	
4-9	Atom designation 1	
10-12	r (= 1, 2, or 3)	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	Vector

Function 108

Same as Function 8 computed for each of the three values of r.

Columns

1-3	108	
4-9	Atom designation 1	
10-12	---	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	Vector

Function 208

Same as Function 8 computed for each atom in a given molecule, each with the three values of r.

Columns

1-3	208	
4-6	a(max), the number of atoms in the parameter list.	
7-9	Molecule designation	
10-12	---	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	Vector

Function 9

The RMS component of thermal displacement of atom 1 along principal axis r, projected on a vector defined by atoms 2 and 3.

Columns

1-3	9
4-9	Atom designation 1
10-12	r (= 1, 2, or 3)
13-18	Atom designation 2 } Vector
19-24	Atom designation 3 } Vector

Function 109

Same as Function 9 computed for the three values of r.

Columns

1-3	109
4-9	Atom designation 1
10-12	---
13-18	Atom designation 2 } Vector
19-24	Atom designation 3 } Vector

Function 209

Same as Function 9 computed for each atom in a given molecule, each with the three values of r.

Columns

1-3	209
4-6	a(max), the number of atoms in the parameter list.
7-9	Molecule designation
10-12	---
13-18	Atom designation 2 } Vector
19-24	Atom designation 3 } Vector

Function 10

Angle between principal axis r of atom 1 and axis i of a cartesian coordinate system. The latter is defined by atoms 2, 3, 4, and 5 as follows: Axis 1 is vector $(\overrightarrow{2,3})$. Axis 2 is (Axis 1)x$(\overrightarrow{4,5})$. Axis 3 is (Axis 1)x(Axis 2).

Columns

1-3	10
4-9	Atom designation 1
10-12	r (= 1, 2, or 3)
13-15	i (= 1, 2, or 3)

Function 10, cont'd

Columns

16-21	Atom designation 2	Vector	Axis defining vectors
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 110

Same as Function 10 computed for the nine combinations of r and i.

Columns

1-3	110		
4-9	Atom designation 1		
10-15	---		
16-21	Atom designation 2	Vector	Axis defining vectors
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 210

Same as Function 10 computed for all atoms in a given molecule, each with the nine combinations of r and i.

Columns

1-3	210		
4-6	a(max), the number of atoms in the parameter list.		
7-9	Molecule designation		
10-15	---		
16-21	Atom designation 2	Vector	Axis defining vectors
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 11

The RMS component of thermal displacement of atom 1 along principal axis r, projected on axis i of a cartesian coordinate system defined by atoms 2, 3, 4, and 5 as described under Function 10.

Columns

1-3	11
4-9	Atom designation 1

Function 11, cont'd

Columns

10-12	r (= 1, 2, or 3)		
13-15	i (= 1, 2, or 3)		
16-21	Atom designation 2	Vector	Axis defining vectors
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 111

Same as Function 11 computed for the nine combinations of r and i.

Columns

1-3	111		
4-9	Atom designation 1		
10-15	---		
16-21	Atom designation 2	Vector	Axis defining vectors
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 211

Same as Function 11 computed for all atoms in a given molecule, each with the nine combinations of r and i.

Columns

1-3	211		
4-6	a(max), the number of atoms in the parameter list.		
7-9	Molecule designation		
10-15	---		
12-21	Atom designation 2	Vector	Axis defining vectors
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 12

The RMS component of thermal displacement of atom 1 in the direction of a vector defined by atoms 2 and 3.

Columns

1-3	12	
4-9	Atom designation 1	
10-15	Atom designation 2	Vector
16-21	Atom designation 3	

Function 13

The RMS radial thermal displacement of an atom.

Columns

1-3	13
4-9	Atom designation

Function 14

Interatomic distance averaged over thermal motion. Second atom is assumed to ride on the first. The function is $\bar{R} = R_o + (\overline{r_2^2} - \overline{\xi_2^2} - \overline{r_1^2} + \overline{\xi_1^2})/2R_o$ where R_o is the uncorrected interatomic distance, $\overline{r_i^2}$ is the mean square radial thermal displacement of atom i, and $\overline{\xi_i^2}$ is the mean square component of displacement of atom i in the direction defined by the interatomic vector

Columns

1-3	14
4-9	Atom designation 1
10-15	Atom designation 2

Function 15

Interatomic distance averaged over thermal motion. Atoms assumed to move independently. The function is $\bar{R} = R_o + (\overline{r_2^2} - \overline{\xi_2^2} + \overline{r_1^2} - \overline{\xi_1^2})/2R_o$ where the symbols are defined as in Function 14 above.

Columns

1-3	15
4-9	Atom designation 1
10-15	Atom designation 2

ERROR INDICATORS

During the course of calculation the program makes many tests for errors which may indicate that the problem is not set up correctly. If the error is one which would probably cause all answers to be incorrect the program stops with an octal number in the storage register, the meaning of which can be found in the table below. If, on the other hand, the error is likely to cause trouble in only one answer then the program does not halt. Instead of the incorrect answer the program puts out "***NG" where NG is an integer, the meaning of which is tabulated below. The program then proceeds with the next function to be computed.

Stops

Storage Register	Subprogram	Meaning
2	SUB2	Record 1 on unit 5 (from OR XLS) is not long enough, or RTT fails 3 times. To try again, push START.
3	SUB3	Record 3 on unit 5 (from OR XLS) is not long enough, or RTT fails 3 times. To try again, push START.
4	SUB4	Number of parameter selection cards specified is too large for storage area, or card reader indicates end-of-file. Replenish cards and start.
5	SUB5	Number of symmetry cards specified is too large, i.e. IC(4) > 48.
17	SUB17	Number of one-punches in parameter selection cards (i.e., K1) is less than the order of the matrix.
30	SUB3	Number of parameter selection words from OR XLS binary tape is larger than the storage area for these words. Storage capacity is 40 words.
77777	SEG2	End of problem as indicated by IN(1) = 0. To read more instruction cards push START.

Error Returns

NG	Subprogram	Meaning
1	ATOM, BETA	The symmetry position specified is negative or greater than the number of symmetry cards.
2	PRE	No PRE routine has been supplied for the function specified.
3	FUN	No FUN routine has been supplied for the function specified.
4	BETA	Temperature factors are not in anisotropic form, i.e., IC(9) < 6.
5	ATOM, BETA	The program is looking for a parameter before the start or beyond the end of the list.
6	STOBB	The cell parameter A(1), A(2), or A(3) ≤ 0.
7	EIGVAL	The eigenvalues are imaginary.
8	EIGVEC	Only null eigenvectors are found.
9	COSVV	One of the vectors is null.
10	FUNXI	The vector is null.
11	SUB 12,14,18	A non-existent function has been specified, i.e. XMODF(IN(1),100) > 20.

COMMON STORAGE

Symbol and Dimension	Description
NG	Error return indicator.
IC(10)	Control card integers.
PM(251)	One row of the variance-covariance matrix associated with the atomic parameters. PM(1) = V_{ii}, PM(2) = V_{ii+1}, etc.
DP(251)	The increments $\Delta p_i = (0.01)V_{ii}^{1/2}$.
DFDP(251)	The derivatives $\partial f/\partial p_i$.
AM(21)	The variance-covariance matrix associated with the six cell parameters. AM(1) = U_{11}, AM(2) = U_{12}, ... AM(6) = U_{16}, AM(7) = U_{22}, ..., etc.
DA(6)	The increments $\Delta a_i = (0.01)U_{ii}^{1/2}$.
DFDA(6)	The derivatives $\partial f/\partial a_i$.
IN(231)	Instruction integers.
TS(3,48)	The translational part of the symmetry information. See below.
IS(2,3,48)	Integers representing the non-translational part of the symmetry information. For example if the Jth symmetry transformation is y-x, -x, 1/3 + z, this information would be stored as follows: TS(1,J) = 0.0 IS(1,1,J) = 2 (for y) IS(2,1,J) = -1 (for -x) TS(2,J) = 0.0 IS(1,2,J) = -1 (for -x) IS(2,2,J) = 0 TS(3,J) = 0.333333 IS(1,3,J) = 3 (for z) IS(2,3,J) = 0
A(6)	The direct lattice parameters a, b, c, cos α, cos β, and cos γ.
AA(3,3)	The metric tensor $\underset{\sim}{g}$ where $g_{ij} = \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j$.
BB(3,3)	The reciprocal metric tensor $\underset{\sim}{g}^{-1}$ where $(g^{-1})_{ij} = \underset{\sim}{b}_i \cdot \underset{\sim}{b}_j$.
F	The computed value of function f to be put out.
FX	The computed value of function f as stored by the subroutines FUNi.
P(300)	The atomic or least squares parameters. The dimension 300 is only a dummy dimension. The true capacity will be greater than this and is determined by the memory size and the length of any subroutines added by the user.

BINARY DECKS SUPPLIED

Identification	Number of Locations	Remarks
Segment 1A (red*)		
NYRBL1		Loader
SEG1A		Program
SEG1A		Transfer card
Segment 1B (orange)		
SEG1B		Fortran II BSS loader
SEG1B		Calling program
SEG1B		Fortran library subroutine
WRITE		SAP subroutine
SEG1B		Fortran II transfer card
Segment 2		
Loader (yellow)		
SEG2		Fortran II BSS loader
Basic program, SAP (yellow)		
SUB2	123	
SUB6	51	
SUBG	125	SUB7, 12, 14, + 18
SUBK	280	SUB1, 3, 4, 15, 16, 17, + 20
READ	37	
SET	1	
HED	1	
PRE	4	
FUN	4	
OUT	1	
	627	
Basic program, Fortran (yellow)		
SEG2	365	Calling program
SUB5	83	
SUB8	101	
SUB10	30	
SUB11	39	
SUB13	403	
SUB19	33	
SUB21	149	
SUBF	1280	Fortran library subroutines
	2483	

*It is suggested that the user reproduce the binary decks in the indicated colors.

Identification	Number of Locations
Arithmetic subprograms, Fortran (yellow)	
SETKX	60
SETKB	60
STOAA	49
STOBB	149
ATOM	231
BETA	296
MM	52
MV	48
VM	46
VV	36
VMV	36
DIFV	33
SUMV	33
COSVV	58
ARCCOS	38
NORM	71
AXES	56
EIGVAL	239
EIGVEC	157
TRACE	32
	1780
Functions 1-6, Fortran (green)	
FUNA	75
FUND	53
HED1	36
PRE1	20
FUN1	19
OUT1	46
HED2	38
PRE2	29
FUN2	19
OUT2	48
HED3	40
PRE3	29
FUN3	122
OUT3	57
HED4	38
PRE4	29
FUN4	25
OUT4	53
HED5	36

FUN5	25

HED6	35
PRE6	38
FUN6	41
OUT6	67
	1018

Identification	Number of Locations
Functions 7-11, Fortran (blue)	
FUNB	71
FUNC	80
FUNX	152
HED7	47
PRE7	18
FUN7	30
OUT7	44
HED8	48
PRE8	32
FUN8	25
OUT8	50
HED9	57

FUN9	24

HED10	53
PRE10	32
FUN10	25
OUT10	60
HED11	62

FUN11	24

	934
Functions 12-15, Fortran (brown)	
FUNR	58
FUNCR	93
FUNXI	113
HED12	51
PRE12	32
FUN12	25
OUT12	50
HED13	39
PRE7	18 (duplicate)
FUN13	24
OUT13	43
HED14	45
PRE14	38
FUN14	36
OUT1	46 (duplicate)
HED15	45

FUN15	36

	792

Identification	Number of Locations			Remarks
Transfer card (red stripe)				
SEG2				Fortran transfer card

Storage requirements, Segment 2

Functions:	1-6	7-11	12-15	1-15
Basic program, SAP	627	627	627	627
Basic program, Fortran	2483	2483	2483	2483
Arithmetic	1780	1780	1780	1780
Functions	1018	934	792	2744
Loader	24	24	24	24
Common (program)	1786	1786	1786	1786
Common (Fortran)	205	205	205	205
Total	7923	7839	7697	9649

```
SEG1A REM SEGMENT TO READ INVERSE MATRIX FROM TAPE                    SEG1A
START EQU 301                REFERS TO OR XLS2                        SEG1A
T68   EQU 4391               REFERS TO OR XLS2                        SEG1A
K2    EQU 32753              REFERS TO OR XLS2                        SEG1A
      ORG 85                                                          SEG1A
A1    REW 5                                                           SEG1A
      REW 6                                                           SEG1A
      TSX RTB,4                                                       SEG1A
      PZE 5                                                           SEG1A
      PZE -PM                                                         SEG1A
      HTR 0                  END OF FILE                              SEG1A
      LDQ PM-START+T68                                                SEG1A
      FMP PM-START+T68                                                SEG1A
      STO SCALE                                                       SEG1A
      RTB 5                                                           SEG1A
A14   TSX RTB,4                                                       SEG1A
      PZE 5                                                           SEG1A
      PZE -PM                                                         SEG1A
      HTR 0                  END OF FILE                              SEG1A
      CLA PM-32512+K2                                                 SEG1A
      STO N                                                           SEG1A
      TNZ A15                                                         SEG1A
      HTR 0                  ORDER OF MATRIX IS ZERO                  SEG1A
A15   RTB 5                                                           SEG1A
A2    RTB 5                                                           SEG1A
      CPY DISC                                                        SEG1A
      TRA A2                                                          SEG1A
      LXD A4,4                                                        SEG1A
A3    RTB 5                                                           SEG1A
      CPY DISC                                                        SEG1A
A4    TXI A5,0,4                                                      SEG1A
      HTR 0                  END OF FILE                              SEG1A
A5    TIX A3,4,1                                                      SEG1A
      TSX RTB,4                                                       SEG1A
      PZE 5                                                           SEG1A
A6    PZE -PM                                                         SEG1A
      HTR 0                  END OF FILE                              SEG1A
```

```
        REW 5                                                   SEG1A
        CLA N                                                   SEG1A
        ADD I1                                                  SEG1A
        LRS 35                                                  SEG1A
        MPY N                                                   SEG1A
        LRS 1                                                   SEG1A
        STQ M                                                   SEG1A
        LXA M,4                                                 SEG1A
        LXA A6,2                                                SEG1A
A7      LDQ SCALE                                               SEG1A
        FMP 0,2                                                 SEG1A
        STO 0,2                                                 SEG1A
        TXI A8,2,-1                                             SEG1A
A8      TIX A7,4,1                                              SEG1A
        CAL N                                                   SEG1A
        SUB I1                                                  SEG1A
        ALS 18                                                  SEG1A
        ADD N                                                   SEG1A
        SLW DELTA                                               SEG1A
        CAL A6                                                  SEG1A
        SUB N                                                   SEG1A
        ALS 18                                                  SEG1A
        ADD A6                                                  SEG1A
        SLW A10                                                 SEG1A
        LXA N,1                                                 SEG1A
A9      SXD X1,1                                                SEG1A
        TSX WTB,4                                               SEG1A
        PZE 6                                                   SEG1A
A10     PZE **                  -INITIAL,0,-(FINAL+1)           SEG1A
        LXD X1,1                                                SEG1A
        TNX A11,1,1                                             SEG1A
        CAL A10                                                 SEG1A
        SUB DELTA                                               SEG1A
        SLW A10                                                 SEG1A
        CAL DELTA                                               SEG1A
        SUB ID1                                                 SEG1A
        SLW DELTA                                               SEG1A
        TRA A9                                                  SEG1A
A11     WEF 6                                                   SEG1A
```

```
       REW 6                                                    SEG1A
A12    RCD                                                      SEG1A
       CPY 0                                                    SEG1A
       TRA A13                                                  SEG1A
       HTR A12                 END OF FILE                      SEG1A
A13    CPY 1                                                    SEG1A
       TRA 0                                                    SEG1A
       REM SUBROUTINE TO STORE BLOCK ON TAPE                    XLS  037
WTB    CLA 1,4                                                  XLS  038
       ADD WTB12                                                XLS  039
       STA WTB3                                                 XLS  040
       STA WTB7                                                 XLS  041
       CLA 1,4                                                  XLS  042
       ADD WTB13                                                XLS  043
       STA WTB6                                                 XLS  044
       STA WTB11                                                XLS  045
WTB1   LXD WTB9,1                                               XLS  046
WTB2   CLA 2,4                                                  XLS  047
       PAX 0,2                                                  XLS  048
       STD WTB5                                                 XLS  049
WTB3   WTB 0                   ADDRESS TO BESET                 XLS  050
WTB4   CPY 0,2                                                  XLS  051
       TXI WTB5,2,-1                                            XLS  052
WTB5   TXH WTB4,2,0            DECREMENT TO BE SET              XLS  053
WTB6   BST 0                   ADDRESS TO BE SET                XLS  054
WTB7   RTB 0                   ADDRESS TO BE SET                XLS  055
       RTT                                                      XLS  056
       NOP                                                      XLS  057
WTB8   CPY WTB10                                                XLS  058
WTB9   TXI WTB8,0,3                                             XLS  059
WTB10  PZE                     READ-BACK COPIED HERE            XLS  060
       IOD                                                      XLS  061
       RTT                                                      XLS  062
       TRA WTB11                                                XLS  063
       TRA 3,4                                                  XLS  064
WTB11  BST 0                   ADDRESS TO BE SET                XLS  065
       TIX WTB2,1,1                                             XLS  066
       HTR WTB1                RTT FAILS 3 TIMES. START TO TRY AGAIN  XLS  067
WTB12  WTB 0                   CONSTANT                         XLS  068
```

```
WTB13 BST 0                    CONSTANT                                    XLS  069
      REM SUBROUTINE TO READ RECORD FROM TAPE                              XLS  070
RTB   CLA 1,4                                                              XLS  071
      ADD RTB7                                                             XLS  072
      STO RTB3                                                             XLS  073
      CLA 1,4                                                              XLS  074
      ADD RTB8                                                             XLS  075
      STO RTB6                                                             XLS  076
RTB1  LXD RTB5,1                                                           XLS  077
RTB2  CLA 2,4                                                              XLS  078
      PAX 0,2                                                              XLS  079
RTB3  RTB 0                    TO BE SET                                   XLS  080
      RTT                                                                  XLS  081
      NOP                                                                  XLS  082
RTB4  CPY 0,2                                                              XLS  083
      TXI RTB4,2,-1                                                        XLS  084
      TRA 3,4                                                              XLS  085
      IOD                                                                  XLS  086
      RTT                                                                  XLS  087
RTB5  TXI RTB6,0,3                                                         XLS  088
      TRA 4,4                                                              XLS  089
RTB6  BST 0                    TO BE SET                                   XLS  090
      TIX RTB2,1,1                                                         XLS  091
      HTR RTB1                 RTT FAILS 3 TIMES. START TO TRY AGAIN.      XLS  092
RTB7  RTB 0                    CONSTANT                                    XLS  093
RTB8  BST 0                    CONSTANT                                    XLS  094
I1    PZE 1                                                                SEG1A
ID1   PZE 1,0,1                                                            SEG1A
SCALE                          SCALE FACTOR FOR MATRIX                     SEG1A
N                              ORDER OF MATRIX                             SEG1A
M                              NUMBER OF MATRIX ELEMENTS                   SEG1A
DELTA                          INCREMENT FOR A10                           SEG1A
X1                             INDEX SAVED HERE                            SEG1A
DISC                           DISCARDS COPIED HERE                        SEG1A
PM                             START OF MAIN STORAGE                       SEG1A
      END A1                                                               SEG1A

CSEG1B   1471 WRB SEGMENT 1B CALLING PROGRAM                               SEG1B101
      COMMONPM                                                             SEG1B103
```

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```
      DIMENSIONPM(1000)                                                 SEG1B105
C     ABOVE DIMENSION IS DUMMY. MATRIX LIMITED ONLY BY MEMORY CAPACITY. SEG1B106
      READ109,N,SCALE                                                   SEG1B107
  109 FORMAT(I9,E9.4)                                                   SEG1B109
      M=(N*(N+1))/2                                                     SEG1B111
      READ115,(PM(I),I=1,M)                                             SEG1B113
  115 FORMAT(8E9.4)                                                     SEG1B115
      DO119I=1,M                                                        SEG1B117
  119 PM(I)=SCALE*PM(I)                                                 SEG1B119
      REWIND6                                                           SEG1B121
      K=1                                                               SEG1B123
      L=N                                                               SEG1B125
      DO207J=1,N                                                        SEG1B201
      CALLWRITE(6,PM(K),L)                                              SEG1B203
      K=K+L                                                             SEG1B205
  207 L=L-1                                                             SEG1B207
      REWIND6                                                           SEG1B209
      END(0,1,0,0,1)                                                    SEG1B211

       REM WRB 1471 SUBROUTINE WRITE(TAPE,LOC,NO.WORDS)
       ORG 0
       FUL
       MZE 0,0,4
       PZE
       PZE WTB13+1
       PZE
       BCD 1WRITE
       PZE A
       ORG 0
       REL
       PZE                    SAVE INDEX 1
       PZE                    SAVE INDEX 2
       PZE                    SAVE INDEX 4
A      SXD A-3,1
       SXD A-2,2
       SXD A-1,4
       CLA 1,4
       STA WTB
       CLA 2,4
```

```
        STA WTB4
        CLA 3,4
        STA WTB2
WTB     CLA 0                   ADDRESS TO BE SET
        ARS 18
        STO WTB10
        ADD WTB12
        STA WTB3
        STA WTB7
        CLA WTB10
        ADD WTB13
        STA WTB6
        STA WTB11
WTB1    LXD WTB9,1
WTB2    LXD 0,4                 ADDRESS TO BE SET
        PXD 0,0
        PDX 0,2
WTB3    WTB 0                   ADDRESS TO BESET
WTB4    CPY 0,2
        TXI WTB5,2,1
WTB5    TIX WTB4,4,1
WTB6    BST 0                   ADDRESS TO BE SET
WTB7    RTB 0                   ADDRESS TO BE SET
        RTT
        NOP
WTB8    CPY WTB10
WTB9    TXI WTB8,0,3
WTB10   PZE                     READ-BACK COPIED HERE
        IOD
        RTT
        TRA WTB11
        LXD A-3,1
        LXD A-2,2
        LXD A-1,4
        TRA 4,4
WTB11   BST 0                   ADDRESS TO BE SET
        TIX WTB2,1,1
        HTR WTB1                RTT FAILS 3 TIMES. START TO TRY AGAIN
WTB12   WTB 0                   CONSTANT
```

```
WTB13 BST 0                    CONSTANT
      END 0

SUB2  REM 1471 WRB READ PARAMETERS FROM XLS BINARY TAPE          SUB2 001
      REM PROGRAM CARD                                           SUB2 002
      FUL                                                        SUB2 003
      MZE 0,0,4                9L                                SUB2 004
      PZE                                                        SUB2 005
      PZE T1+1                                                   SUB2 006
      PZE                                                        SUB2 007
      BCD 1SUB2                                                  SUB2 008
      PZE SUB2                 7R                                SUB2 009
      REM SUBROUTINE SUB2(P,IC)                                  SUB2 010
      ORG 0                                                      SUB2 011
      REL                                                        SUB2 012
SUB2  SXD X1,1                                                   SUB2 013
      SXD X2,2                                                   SUB2 014
      SXD X4,4                                                   SUB2 015
      CLA 1,4                                                    SUB2 016
      STA S2U                                                    SUB2 017
      STA S2AA                                                   SUB2 018
      CLA 2,4                                                    SUB2 019
      SUB I1                                                        20
      STA S2AC                                                      21
      SUB I5                                                        22
      STA S2AF                                                   SUB2 023
      SUB I1                                                     SUB2 024
      STA S2AD                                                   SUB2 025
      SUB I1                                                     SUB2 026
      STA S2AG                                                   SUB2 027
      SUB I1                                                     SUB2 028
      STA S2AE                                                   SUB2 029
S2A   LXA I3,1                                                   SUB2 030
S2B   REW 5                                                      SUB2 031
      RTB 5                                                      SUB2 032
      RTT                                                        SUB2 033
      NOP                                                        SUB2 034
      LXA C1,2                                                   SUB2 035
S2C   CPY S3                                                     SUB2 036
```

```
        TRA S2E                                                  SUB2 037
S2D     HPR 2                 END OF FIEL OR RECORD              SUB2 038
        TRA S2D                                                  SUB2 039
S2E     TIX S2C,2,1                                              SUB2 040
        LXA C2,2                                                 SUB2 041
S2F     CPY S11                                                  SUB2 042
        TRA S2H                                                  SUB2 043
S2G     HPR 2                                                    SUB2 044
        TRA S2G                                                  SUB2 045
S2H     TIX S2F,2,1                                              SUB2 046
        LXA C3,2                                                 SUB2 047
S2I     CPY T61                                                  SUB2 048
        TRA S2K                                                  SUB2 049
S2J     HPR 2                                                    SUB2 050
        TRA S2J                                                  SUB2 051
S2K     TIX S2I,2,1                                              SUB2 052
        LXA C4,2                                                 SUB2 053
S2L     CPY T6                                                   SUB2 054
        TRA S2N                                                  SUB2 055
S2M     HPR 2                                                    SUB2 056
        TRA S2M                                                  SUB2 057
S2N     TIX S2L,2,1                                              SUB2 058
        LXA C5,2                                                 SUB2 059
S2O     CPY T5                                                   SUB2 060
        TRA S2Q                                                  SUB2 061
S2P     HPR 2                                                    SUB2 062
        TRA S2P                                                  SUB2 063
S2Q     TIX S2O,2,1                                              SUB2 064
        CLA T5                                                   SUB2 065
        SUB C6                                                   SUB2 066
        PAX 0,2                                                  SUB2 067
S2R     CPY T1                                                   SUB2 068
        TRA S2T                                                  SUB2 069
S2S     HPR 2                                                    SUB2 070
        TRA S2S                                                  SUB2 071
S2T     TIX S2R,2,1                                              SUB2 072
        PXD 0,0                                                  SUB2 073
        PDX 0,4                                                  SUB2 074
        LXA S11,2                                                SUB2 075
```

```
        TXI  S2U,2,1                                    SUB2 076
S2U     CPY  **,4              P(1)                     SUB2 077
        TXI  S2W,4,1                                    SUB2 078
S2V     HPR  2                                          SUB2 079
        TRA  S2V                                        SUB2 080
S2W     TIX  S2U,2,1                                    SUB2 081
        CLA  T61                                        SUB2 082
        SUB  T6                                         SUB2 083
        TZE  S2AA                                       SUB2 084
        PAX  0,2                                        SUB2 085
S2X     CPY  T1                                         SUB2 086
        TRA  S2Z                                        SUB2 087
S2Y     HPR  2                                          SUB2 088
        TRA  S2Y                                        SUB2 089
S2Z     TIX  S2X,2,1                                    SUB2 090
S2AA    CPY  **,4              P(1)                     SUB2 091
        TXI  S2AA,4,1                                   SUB2 092
        HTR  0                                          SUB2 093
S2AB    IOD                                             SUB2 095
        RTT                                             SUB2 096
        TRA  S2AH                                       SUB2 097
        PXD  0,4                                        SUB2 098
S2AC    STO  **                IC(2)                    SUB2 981
        LXA  S11,4                                      SUB2 099
        TXI  S2AI,4,3                                   SUB2 100
S2AI    PXD  0,4                                        SUB2 101
S2AD    STO  **                IC(8)                    SUB21011
        TXI  S2AJ,4,3                                   SUB2 102
S2AJ    PXD  0,4                                        SUB2 103
S2AE    STO  **                IC(10)                   SUB21031
        LDQ  S3                                         SUB2 104
        MPY  I5                                         SUB2 105
        LLS  18                                         SUB2 106
S2AF    STQ  **                IC(7)                    SUB2 107
S2AG    STQ  **                IC(9)                    SUB2 108
        LXD  X1,1                                       SUB2 109
        LXD  X2,2                                       SUB2 110
        LXD  X4,4                                       SUB2 111
        TRA  3,4                                        SUB2 112
```

```
S2AH   TIX S2B,1,1                                                    SUB2 113
       HPR 2                 RTT FAILS 3 TIMES. START                 SUB2 114
       TRA S2A               TO TRY AGAIN                             SUB2 115
L1     EQU 301               455(8) LOC START IN XLS2                 SUB2 116
L2     EQU 4295              10307(8) LOC S3 IN XLS2                  SUB2 117
L3     EQU 4304              10320(8) LOC S11 IN XLS2                 SUB2 118
L4     EQU 4308              10324(8) LOC T61 IN XLS2                 SUB2 119
L5     EQU 4309              10325(8) LOC T6 IN XLS2                  SUB2 120
L6     EQU 4437              10525(8) LOC T5 IN XLS2                  SUB2 121
I1     PZE 1                                                          SUB2 122
I3     PZE 3                                                          SUB2 123
I5     PZE 5                                                          SUB2 124
C1     PZE L2-L1+1                                                    SUB2 125
C2     PZE L3-L2                                                      SUB2 126
C3     PZE L4-L3                                                      SUB2 127
C4     PZE L5-L4                                                      SUB2 128
C5     PZE L6-L5                                                      SUB2 129
C6     PZE L6                                                         SUB2 130
X1                           INDEX SAVED HERE                         SUB2 131
X2                           INDEX SAVED HERE                         SUB2 132
X4                           INDEX SAVED HERE                         SUB2 133
S3                           XLS2 SYMM OR ANIS INDICATOR              SUB2 134
S11                          XLS2 NO. OF SCALE FACTORS                SUB2 135
T61                          XLS2 COMP LOC SYMM CODE                  SUB2 136
T6                           XLS2 COMP LOC ATOM PARATETERS            SUB2 137
T5                           XLS2 LAST LOC USED BY CODE               SUB2 138
T1                           DISCARDS COPIED HERE                     SUB2 139
       END 0                                                          SUB2 140

SUB6   REM 1471 WRB DECODE SYMMETRY INFORMATION                       SUB6 001
       REM PROGRAM CARD                                               SUB6 002
       FUL                                                            SUB6 003
       MZE 0,0,4             9L                                       SUB6 004
       PZE                                                            SUB6 005
       PZE TEMP+1                                                     SUB6 006
       PZE                                                            SUB6 007
       BCD 1SUB6                                                      SUB6 008
       PZE SUB6              7R                                       SUB6 009
       REM SUBROUTINE SUB6(1,1,K) TO DECODE SYMM CARD K               SUB6 010
```

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```
        REL                                                     SUB6 011
        ORG 0                                                   SUB6 012
SUB6    SXD X1,1                                                SUB6 013
        SXD X4,4                                                SUB6 014
        CLA 1,4                                                 SUB6 015
        STA S6D                                                 SUB6 016
        STA S6H                                                 SUB6 017
        PXD 0,0                                                 SUB6 018
        PDX 0,1                                                 SUB6 019
S6A     CAL F2,4            FROM FORMAT IN SUB5                 SUB6 020
        ALS 12                                                  SUB6 021
        ANA MASK                                                SUB6 022
        TZE S6B                                                 SUB6 023
        SUB D6                                                  SUB6 024
        SLW TEMP                                                SUB6 025
        CAL F2,4            FROM FORMAT IN SUB5                 SUB6 026
        ANA MASK1                                               SUB6 027
        TNZ S6C                                                 SUB6 028
        CLS TEMP                                                SUB6 029
        TRA S6D                                                 SUB6 030
S6B     PXD 0,0                                                 SUB6 031
        TRA S6D                                                 SUB6 032
S6C     CLA TEMP                                                SUB6 033
S6D     STO **,1            LOC IS(1,1,K)                       SUB6 034
        TXI S6E,1,1                                             SUB6 035
S6E     CAL F2+1,4          FROM FORMAT IN SUB5                 SUB6 036
        ARS 12                                                  SUB6 037
        ANA MASK                                                SUB6 038
        TZE S6F                                                 SUB6 039
        SUB D6                                                  SUB6 040
        SLW TEMP                                                SUB6 041
        CAL F2,4            FROM FORMAT IN SUB5                 SUB6 042
        ANA MASK2                                               SUB6 043
        TNZ S6G                                                 SUB6 044
        CLS TEMP                                                SUB6 045
        TRA S6H                                                 SUB6 046
S6F     PXD 0,0                                                 SUB6 047
        TRA S6H                                                 SUB6 048
S6G     CLA TEMP                                                SUB6 049
```

```
S6H    STO **,1                LOC IS(1,1,K)                                SUB6 050
       TXI S6I,1,1                                                          SUB6 051
S6I    TXH S6J,1,5                                                          SUB6 052
       TXI S6A,4,-2                                                         SUB6 053
S6J    LXD X1,1                                                             SUB6 054
       LXD X4,4                                                             SUB6 055
       TRA 2,4                                                              SUB6 056
MASK   OCT 000017000000                                                     SUB6 057
MASK1  OCT 000000400000                                                     SUB6 058
MASK2  OCT 000000000040                                                     SUB6 059
D4     PZE 0,0,4                                                            SUB6 060
X1                             INDEX SAVED HERE                             SUB6 061
X4                             INDEX SAVED HERE                             SUB6 062
TEMP                                                                        SUB6 063
F2     EQU 22                  SECOND FORMAT WORD LESS TSX SUB6             SUB6 064
       END 0                                                                SUB6 065

SUBG   REM 1471 WRB COMPUTED SUBROUTINE ENTRIES                             SUBG 001
       REM PROGRAM CARD                                                     SUBG 002
       FUL                                                                  SUBG 003
       MZE 0,0,10              9L                                           SUBG 004
       PZE                                                                  SUBG 005
       PZE X4+1,0,82                                                        SUBG 006
       PZE                                                                  SUBG 007
       BCD 1SUB7                                                            SUBG 008
       PZE SUB7                                                             SUBG 009
       BCD 1SUB12                                                           SUBG 010
       PZE SUB12                                                            SUBG 011
       BCD 1SUB14                                                           SUBG 012
       PZE SUB14                                                            SUBG 013
       BCD 1SUB18                                                           SUBG 014
       PZE SUB18               4R                                           SUBG 015
       ORG 0                                                                SUBG 016
       REL                                                                  SUBG 017
SETA   BCD 1SETA                                                            SUBG 018
SETP   BCD 1SETP                                                            SUBG 019
       BCD 1HED20                                                           SUBG 020
       BCD 1HED19                                                           SUBG 021
       BCD 1HED18                                                           SUBG 022
```

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```
        BCD 1HED17
        BCD 1HED16
        BCD 1HED15
        BCD 1HED14
        BCD 1HED13
        BCD 1HED12
        BCD 1HED11
        BCD 1HED10
        BCD 1HED9
        BCD 1HED8
        BCD 1HED7
        BCD 1HED6
        BCD 1HED5
        BCD 1HED4
        BCD 1HED3
        BCD 1HED2
        BCD 1HED1
HED     BSS 0
        BCD 1PRE20
        BCD 1PRE19
        BCD 1PRE18
        BCD 1PRE17
        BCD 1PRE16
        BCD 1PRE14          SAME AS PRE15
        BCD 1PRE14
        BCD 1PRE7           SAME AS PRE 13
        BCD 1PRE12
        BCD 1PRE10          SAME AS PRE11
        BCD 1PRE10
        BCD 1PRE8           SAME AS PRE9
        BCD 1PRE8
        BCD 1PRE7
        BCD 1PRE6
        BCD 1PRE3           SAME AS PRE5
        BCD 1PRE4
        BCD 1PRE3
        BCD 1PRE2
        BCD 1PRE1
PRE     BSS 0
```

```
SUBG 023
SUBG 024
SUBG 025
SUBG 026
SUBG 027
SUBG 028
SUBG 029
SUBG 030
SUBG 031
SUBG 032
SUBG 033
SUBG 034
SUBG 035
SUBG 036
SUBG 037
SUBG 038
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SUBG 052
SUBG 053
SUBG 054
SUBG 055
SUBG 056
SUBG 057
SUBG 058
SUBG 059
SUBG 060
SUBG 061
```

```
        BCD 1FUN20                                          SUBG 062
        BCD 1FUN19                                          SUBG 063
        BCD 1FUN18                                          SUBG 064
        BCD 1FUN17                                          SUBG 065
        BCD 1FUN16                                          SUBG 066
        BCD 1FUN15                                          SUBG 067
        BCD 1FUN14                                          SUBG 068
        BCD 1FUN13                                          SUBG 069
        BCD 1FUN12                                          SUBG 070
        BCD 1FUN11                                          SUBG 071
        BCD 1FUN10                                          SUBG 072
        BCD 1FUN9                                           SUBG 073
        BCD 1FUN8                                           SUBG 074
        BCD 1FUN7                                           SUBG 075
        BCD 1FUN6                                           SUBG 076
        BCD 1FUN5                                           SUBG 077
        BCD 1FUN4                                           SUBG 078
        BCD 1FUN3                                           SUBG 079
        BCD 1FUN2                                           SUBG 080
        BCD 1FUN1                                           SUBG 081
FUN     BSS 0                                               SUBG 082
        BCD 1OUT20                                          SUBG 083
        BCD 1OUT19                                          SUBG 084
        BCD 1OUT18                                          SUBG 085
        BCD 1OUT17                                          SUBG 086
        BCD 1OUT16                                          SUBG 087
        BCD 1OUT1          SAME AS OUT15                    SUBG 088
        BCD 1OUT1          SAME AS OUT14                    SUBG 089
        BCD 1OUT13                                          SUBG 090
        BCD 1OUT12                                          SUBG 091
        BCD 1OUT10         SAME AS OUT11                    SUBG 092
        BCD 1OUT10                                          SUBG 093
        BCD 1OUT8          SAME AS OUT9                     SUBG 094
        BCD 1OUT8                                           SUBG 095
        BCD 1OUT7                                           SUBG 096
        BCD 1OUT6                                           SUBG 097
        BCD 1OUT3          SAME AS OUT5                     SUBG 098
        BCD 1OUT4                                           SUBG 099
        BCD 1OUT3                                           SUBG 100
```

```
        BCD 1OUT2                                                SUBG 101
        BCD 1OUT1                                                SUBG 102
OUT     BSS 0                                                    SUBG 103
SUB7    SXD X2,2                                                 SUBG 104
        SXD X4,4                                                 SUBG 105
        CLM                                                      SUBG 106
        LDQ IN                                                   SUBG 107
        LLS 0                                                    SUBG 108
        DVP D100                                                 SUBG 109
        PDX 0,2                                                  SUBG 110
        TXH EXIT,2,20                                            SUBG 111
        TSX HEDI,4                                               SUBG 112
        TRA EXIT                                                 SUBG 113
HEDI    TRA HED,2                                                SUBG 114
SUB12   SXD X2,2                                                 SUBG 115
        SXD X4,4                                                 SUBG 116
        TSX SETA,4                                               SUBG 117
        TSX SETP,4                                               SUBG 118
        LXD IN,2                                                 SUBG 119
        TXH EXNG,2,20                                            SUBG 120
        TSX FUNI,4                                               SUBG 121
        TRA EXIT                                                 SUBG 122
FUNI    TRA FUN,2                                                SUBG 123
SUB14   SXD X2,2                                                 SUBG 124
        SXD X4,4                                                 SUBG 125
        LXD IN,2                                                 SUBG 126
        TXH EXNG,2,20                                            SUBG 127
        TSX PREI,4                                               SUBG 128
        TRA EXIT                                                 SUBG 129
PREI    TRA PRE,2                                                SUBG 130
SUB18   SXD X2,2                                                 SUBG 131
        SXD X4,4                                                 SUBG 132
        LXD IN,2                                                 SUBG 133
        TXH EXNG,2,20                                            SUBG 134
        TSX OUTI,4                                               SUBG 135
        TRA EXIT                                                 SUBG 136
OUTI    TRA OUT,2                                                SUBG 137
EXNG    CLA D11                                                  SUBG 138
        STO NG                                                   SUBG 139
```

```
EXIT  LXD X2,2                                                    SUBG 140
      LXD X4,4                                                    SUBG 141
      TRA 1,4                                                     SUBG 142
D11   PZE 0,0,11                                                  SUBG 143
D100  PZE 0,0,100                                                 SUBG 144
IN    SYN 31765             REFERS TO COMMON STORAGE              SUBG 145
NG    SYN 32562             REFERS TO COMMON STORAGE              SUBG 146
X2                          INDEX STORED HERE                     SUBG 147
X4                          INDEX STORED HERE                     SUBG 148
      END 0                                                       SUBG 149

SUBK  REM 1471 WRB KEY WORD SUBROUTINES                           SUBK 001
      REM PROGRAM CARD                                            SUBK 002
      FUL                                                         SUBK 003
      MZE 0,0,16            9L                                    SUBK 004
      PZE                                                         SUBK 005
      PZE X4+1                                                    SUBK 006
      PZE                                                         SUBK 007
      BCD 1SUB1                                                   SUBK 008
      PZE SUB1                                                    SUBK 009
      BCD 1SUB3                                                   SUBK 010
      PZE SUB3                                                    SUBK 011
      BCD 1SUB4                                                   SUBK 012
      PZE SUB4                                                    SUBK 013
      BCD 1SUB15                                                  SUBK 014
      PZE SUB15                                                   SUBK 015
      BCD 1SUB16                                                  SUBK 016
      PZE SUB16                                                   SUBK 017
      BCD 1SUB17                                                  SUBK 018
      PZE SUB17                                                   SUBK 019
      BCD 1SUB20                                                  SUBK 020
      PZE SUB20             1R                                    SUBK 021
      REM SUBROUTINE SUB1 TO CLEAR K2                             SUBK 022
      ORG 0                                                       SUBK 023
      REL                                                         SUBK 024
SUB1  SXD X1,1                                                    SUBK 025
      LXA IDIMK,1                                                 SUBK 026
S1A   STZ K2+DIMK,1                                               SUBK 027
      TIX S1A,1,1                                                 SUBK 028
```

```
      LXD X1,1                                                          SUBK 029
      TRA 1,4                                                           SUBK 030
      REM SUBROUTINE SUB3(IC(5)) TO READ K1 AND IC(5) FROM TAPE         SUBK 031
SUB3  SXD X1,1                                                          SUBK 032
      SXD X2,2                                                          SUBK 033
      CLA 1,4                                                           SUBK 034
      STA S3K                                                           SUBK 035
      RTB 5                                                             SUBK 036
S3A   LXA I3,1                                                          SUBK 037
S3B   RTB 5                                                             SUBK 038
      RTT                                                               SUBK 039
      NOP                                                               SUBK 040
      LXA IDIS,2                                                        SUBK 041
S3C   CPY K1                                                            SUBK 042
      TRA S3E                                                           SUBK 043
S3D   HPR 3                END OF FILE OR RECORD                        SUBK 044
      TRA S3D                                                           SUBK 045
S3E   TIX S3C,2,1                                                       SUBK 046
      LXA IDIMK,2                                                       SUBK 047
S3F   CPY K1+DIMK,2                                                     SUBK 048
      TRA S3H                                                           SUBK 049
S3G   HPR 3                END OF RECORD                                SUBK 050
      TRA S3G                                                           SUBK 051
S3H   TIX S3F,2,1                                                       SUBK 052
      CPY NK                                                            SUBK 053
      CPY N                                                             SUBK 054
      TRA S3J                                                           SUBK 055
S3I   HPR 3                END OF RECORD                                SUBK 056
      TRA S3I                                                           SUBK 057
S3J   CPY K2                                                            SUBK 058
      TRA S3J                                                           SUBK 059
      HPR 3                                                             SUBK 060
      IOD                                                               SUBK 061
      RTT                                                               SUBK 062
      TRA S3O                                                           SUBK 063
      LXA N,1                                                           SUBK 064
      PXD 0,1                                                           SUBK 065
S3K   STO **               LOC IC(5)                                    SUBK 651
      CLA NK                                                            SUBK 066
```

```
        ADD LOCK1                                                       SUBK 067
        STA S3N                                                         SUBK 068
        LXA NK,1                                                        SUBK 069
        SXD NK,1                                                        SUBK 070
        TXL S3M,1,DIMK                                                  SUBK 071
S3L     HPR 24                  NK GREATER THAN DIMK                    SUBK 072
        TRA S3L                                                         SUBK 073
S3M     CAL K1+DIMK,1                                                   SUBK 074
S3N     SLW **,1                NK+LOCK1                                SUBK 075
        TIX S3M,1,1                                                     SUBK 076
        LXD X1,1                                                        SUBK 077
        LXD X2,2                                                        SUBK 078
        REW 5                                                           SUBK 079
        TRA 2,4                                                         SUBK 080
S3O     BST 5                                                           SUBK 081
        TIX S3B,1,1                                                     SUBK 082
        HPR 3                   RTT FAILS 3 TIMES.                      SUBK 083
        TRA S3A                 START TO TRY AGAIN                      SUBK 084
        REM SUBROUTINE SUB4(IC(6)) TO READ K1 FROM CARDS                SUBK 085
SUB4    SXD X1,1                                                        SUBK 086
        SXD X2,2                                                        SUBK 087
        CAL 1,4                                                         SUBK 088
        STA S4A                                                         SUBK 089
S4A     CLA **                  LOC IC(6)                               SUBK 090
        TZE S4F                                                         SUBK 091
        ALS 1                                                           SUBK 092
        STD NK                                                          SUBK 093
        PDX 0,1                                                         SUBK 094
        ARS 18                                                          SUBK 095
        ADD LOCK1                                                       SUBK 096
        STA S4D                                                         SUBK 097
        ADD I1                                                          SUBK 098
        STA S4E                                                         SUBK 099
        TXL S4C,1,DIMK                                                  SUBK 100
S4B     HPR 4                                                           SUBK 101
        TRA S4B                                                         SUBK 102
S4C     LXA I9,2                                                        SUBK 103
        RCD                                                             SUBK 104
S4D     CPY **,1                NK+LOCK1                                SUBK 105
```

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```
        TRA S4E                                                         SUBK 106
        HPR 4                  END OF FIEL                              SUBK 107
        TRA S4C                                                         SUBK 108
S4E     CPY **,1               NK+LOCK1+1                               SUBK 109
        TIX S4D,2,1                                                     SUBK 110
        TIX S4C,1,2                                                     SUBK 111
        TRA S4H                                                         SUBK 112
S4F     LXA IDIMK,1                                                     SUBK 113
        SXD NK,1                                                        SUBK 114
        PXD 0,0                                                         SUBK 115
        COM                                                             SUBK 116
S4G     SLW K1+DIMK,1                                                   SUBK 117
        TIX S4G,1,1                                                     SUBK 118
S4H     LXD X1,1                                                        SUBK 119
        LXD X2,2                                                        SUBK 120
        TRA 2,4                                                         SUBK 121
        REM SUBROUTINE SUB15(K3) TO STORE SECONDARY KEY WORDS           SUBK 122
        REM     STORES K3(1) ONE BITS STARTING WITH K3(2) BIT           SUBK 123
        REM     OF K3(3) WORD                                           SUBK 124
SUB15   CAL 1,4                                                         SUBK 125
        STA S15A                                                        SUBK 126
        SUB I1                                                          SUBK 127
        STA S15B                                                        SUBK 128
        SUB I1                                                          SUBK 129
        STA S15C                                                        SUBK 130
S15A    CLA **                 LOC K3(1)                                SUBK 131
        ARS 18                                                          SUBK 132
        STA S15D                                                        SUBK 133
S15B    CLA **                 LOC K3(2)                                SUBK 134
        ARS 18                                                          SUBK 135
        STA S15E                                                        SUBK 136
S15C    CLA **                 LOC K3(3)                                SUBK 137
        ARS 18                                                          SUBK 138
        ADD LOCK2                                                       SUBK 139
        STA S15G                                                        SUBK 140
        SUB I1                                                          SUBK 141
        STA S15F                                                        SUBK 142
        PXD 0,0                                                         SUBK 143
        LRS 35                                                          SUBK 144
```

```
      COM
S15D  ARS **                K3(1)
      COM
S15E  LRS **                K3(2)
S15F  ORS **                K3(3)+LOCK2-1
      LLS 36
S15G  ORS **                K3(3)+LOCK2
      TRA 2,4
      REM SUBROUTINE SUB16 TO INITIALIZE SUB17
SUB16 CLA NK
      STD XWORD
      ARS 18
      ADD LOCK1
      STA S17B
      CLA NK
      ARS 18
      ADD LOCK2
      STA S17G
      CLA D36
      STD XBIT
      CAL K1
      SLW TK1
      CAL K2
      SLW TK2
      TRA 1,4
      REM FUNCTION SUB17 TO TEST KEY WORDS
SUB17 SXD X1,1
      LXD XBIT,1
      TIX S17C,1,1
      LXD XWORD,1
      TIX S17B,1,1
S17A  HPR 71                N AND KEY WORDS DISAGREE
      TRA S17A
S17B  CAL **,1              NK+LOCK1 SET BY SUB16
      SLW TK1
S17G  CAL **,1              NK+LOCK2 SET BY SUB16
      SLW TK2
      SXD XWORD,1
      LXD D36,1
```

```
S17C  SXD XBIT,1                                                    SUBK 184
      CAL TK1                                                       SUBK 185
      PBT                                                           SUBK 186
      TRA S17E                                                      SUBK 187
      ALS 1                                                         SUBK 188
      SLW TK1                                                       SUBK 189
      CAL TK2                                                       SUBK 190
      PBT                                                           SUBK 191
      TRA S17D                                                      SUBK 192
      ALS 1                                                         SUBK 193
      SLW TK2                                                       SUBK 194
      CLA ONE                                                       SUBK 195
      TRA S17F                                                      SUBK 196
S17D  ALS 1                                                         SUBK 197
      SLW TK2                                                       SUBK 198
      CLA ONE                                                       SUBK 199
      CHS                                                           SUBK 200
      TRA S17F                                                      SUBK 201
S17E  ALS 1                                                         SUBK 202
      SLW TK1                                                       SUBK 203
      CAL TK2                                                       SUBK 204
      ALS 1                                                         SUBK 205
      SLW TK2                                                       SUBK 206
      PXD 0,0                                                       SUBK 207
S17F  LXD X1,1                                                      SUBK 208
      TRA 2,4                                                       SUBK 209
      REM SUBROUTINE SUB20                                          SUBK 210
SUB20 REW 5                                                         SUBK 211
      RTB 5                                                         SUBK 212
      TRA 1,4                                                       SUBK 213
      REM CONSTANTS AND TEMPORARIES                                 SUBK 214
DIMK  EQU 40                DIMENSION K1 AND K2                     SUBK 215
L1    EQU 256               WORDS IN XLS TAPE RECORD 3              SUBK 216
L2    EQU 16                WORDS IN XLS INTERSEGMENT STORAGE       SUBK 217
IDIS  PZE L1-L2-DIMK        WORDS TO BE DISCARDED FROM TAPE         SUBK 218
IDIMK PZE DIMK                                                      SUBK 219
I1    PZE 1                                                         SUBK 220
I3    PZE 3                                                         SUBK 221
I9    PZE 9                                                         SUBK 222
```

```
D36    PZE 0,0,36                                                    SUBK 223
ONE    DEC 1.0                                                       SUBK 224
LOCK1  PZE K1                                                        SUBK 225
LOCK2  PZE K2                                                        SUBK 226
K1     BSS DIMK                PRIMARY KEY WORDS                     SUBK 227
K2     BSS DIMK                DECONDARY KEY WORDS                   SUBK 228
TK1                            CURRENT K1                            SUBK 229
TK2                            CURRENT K2                            SUBK 230
XWORD                          KEY WORD COUNTER SAVED                SUBK 231
XBIT                           BIT COUNTER SAVED                     SUBK 232
NK                             NUMBER OF KEY WORDS USED              SUBK 233
N                              ORDER OF MATRIX                       SUBK 234
X1                             IDEX SAVED HERE                       SUBK 235
X2                             IDEX SAVED HERE                       SUBK 236
X4                             IDEX SAVED HERE                       SUBK 237
       END 0                                                         SUBK 238

       REM WRB 1471 SUBROUTINE READ(TAPE,LOC)
       ORG 0
       FUL
       MZE 0,0,4
       PZE
       PZE RTB9+1
       PZE
       BCD 1READ
       PZE A
       ORG 0
       REL
       PZE                     SAVE INDEX 1
       PZE                     SAVE INDEX 2
       PZE                     SAVE INDEX 4
A      SXD A-3,1
       SXD A-2,2
       SXD A-1,4
       CLA 1,4
       STA RTB
       CLA 2,4
       STA RTB4
RTB    CLA 0                   ADDRESS TO BE SET
```

```
        ARS 18
        STO RTB9
        ADD RTB7
        STO RTB3
        CLA RTB9
        ADD RTB8
        STO RTB6
RTB1    LXD RTB5,1
RTB2    PXD 0,0
        PDX 0,2
RTB3    RTB 0                   TO BE SET
        RTT
        NOP
RTB4    CPY 0,2
        TXI RTB4,2,1
        HTR RTB3                END OF FILE
        IOD
        RTT
RTB5    TXI RTB6,0,3
        LXD A-3,1
        LXD A-2,2
        LXD A-1,4
        TRA 3,4
RTB6    BST 0                   TO BE SET
        TIX RTB2,1,1
        HTR RTB1                RTT FAILS 3 TIMES. START TO TRY AGAIN.
RTB7    RTB 0                   CONSTANT
RTB8    BST 0                   CONSTANT
RTB9    PZE                     TAPE NUMBER
        END 0

SET     REM 1471 WRB DUMMY ROUTINES. MAY BE SUPERCEDED BY USER.          SET  001
        REM PROGRAM CARD                                                 SET  002
        FUL                                                              SET  003
        MZE 0,0,6               9L                                       SET  005
        PZE                                                              SET  006
        PZE SET+1                                                        SET  007
        PZE                                                              SET  008
        BCD 1SETA                                                        SET  009
```

```
        PZE SET                                                         SET  010
        BCD 1SETP                                                       SET  011
        PZE SET                 6R                                      SET  012
        REM SUBROUTINES SETA AND SETP                                   SET  013
        REL                                                             SET  014
        ORG 0                                                           SET  015
SET     TRA 1,4                                                         SET  016
        END 0                                                           SET  017

HED     REM 1471 WRB DUMMY ROUTINES TO BE SUPERCEDED                    HED  001
        REM PROGRAM CARD 1                                              HED  002
        FUL                                                             HED  003
        MZE 0,0,22              9L                                      HED  004
        PZE                                                             HED  005
        PZE HED+1                                                       HED  006
        PZE                                                             HED  007
        BCD 1HED1                                                       HED  008
        PZE HED                                                         HED  009
        BCD 1HED2                                                       HED  010
        PZE HED                                                         HED  011
        BCD 1HED3                                                       HED  012
        PZE HED                                                         HED  013
        BCD 1HED4                                                       HED  014
        PZE HED                                                         HED  015
        BCD 1HED5                                                       HED  016
        PZE HED                                                         HED  017
        BCD 1HED6                                                       HED  018
        PZE HED                                                         HED  019
        BCD 1HED7                                                       HED  020
        PZE HED                                                         HED  021
        BCD 1HED8                                                       HED  022
        PZE HED                                                         HED  023
        BCD 1HED9                                                       HED  024
        PZE HED                                                         HED  025
        BCD 1HED10                                                      HED  026
        PZE HED                 12R                                     HED  027
        REM PROGRAM CARD 2                                              HED  028
        MZE 0,0,20              9L                                      HED  029
        PZE                                                             HED  030
```

```
        BCD 1HED11                                                      HED  031
        PZE HED                                                         HED  032
        BCD 1HED12                                                      HED  033
        PZE HED                                                         HED  034
        BCD 1HED13                                                      HED  035
        PZE HED                                                         HED  036
        BCD 1HED14                                                      HED  037
        PZE HED                                                         HED  038
        BCD 1HED15                                                      HED  039
        PZE HED                                                         HED  040
        BCD 1HED16                                                      HED  041
        PZE HED                                                         HED  042
        BCD 1HED17                                                      HED  043
        PZE HED                                                         HED  044
        BCD 1HED18                                                      HED  045
        PZE HED                                                         HED  046
        BCD 1HED19                                                      HED  047
        PZE HED                                                         HED  048
        BCD 1HED20                                                      HED  049
        PZE HED                 11R                                     HED  050
        REM DUMMY SUBROUTINE HED                                        HED  051
        REL                                                             HED  052
        ORG 0                                                           HED  053
HED     TRA 1,4                                                         HED  054
        END 0                                                           HED  055

PRE     REM 1471 WRB DUMMY ROUTINES TO BE SUPERCEDED                    PRE  001
        REM PROGRAM CARD 1                                              PRE  002
        FUL                                                             PRE  003
        MZE 0,0,22              9L                                      PRE  004
        PZE                                                             PRE  005
        PZE D2+1                                                        PRE  006
        PZE                                                             PRE  007
        BCD 1PRE1                                                       PRE  008
        PZE PRE                                                         PRE  009
        BCD 1PRE2                                                       PRE  010
        PZE PRE                                                         PRE  011
        BCD 1PRE3                                                       PRE  012
        PZE PRE                                                         PRE  013
```

```
BCD 1PRE4                                                    PRE  014
PZE PRE                                                      PRE  015
BCD 1PRE5                                                    PRE  016
PZE PRE                                                      PRE  017
BCD 1PRE6                                                    PRE  018
PZE PRE                                                      PRE  019
BCD 1PRE7                                                    PRE  020
PZE PRE                                                      PRE  021
BCD 1PRE8                                                    PRE  022
PZE PRE                                                      PRE  023
BCD 1PRE9                                                    PRE  024
PZE PRE                                                      PRE  025
BCD 1PRE10                                                   PRE  026
PZE PRE                12R                                   PRE  027
REM PROGRAM CARD 2                                           PRE  028
MZE 0,0,20             9L                                    PRE  029
PZE PRE                                                      PRE  030
BCD 1PRE11                                                   PRE  031
PZE PRE                                                      PRE  032
BCD 1PRE12                                                   PRE  033
PZE PRE                                                      PRE  034
BCD 1PRE13                                                   PRE  035
PZE PRE                                                      PRE  036
BCD 1PRE14                                                   PRE  037
PZE PRE                                                      PRE  038
BCD 1PRE15                                                   PRE  039
PZE PRE                                                      PRE  040
BCD 1PRE16                                                   PRE  041
PZE PRE                                                      PRE  042
BCD 1PRE17                                                   PRE  043
PZE PRE                                                      PRE  044
BCD 1PRE18                                                   PRE  045
PZE PRE                                                      PRE  046
BCD 1PRE19                                                   PRE  047
PZE PRE                                                      PRE  048
BCD 1PRE20                                                   PRE  049
PZE PRE                11R                                   PRE  050
REM DUMMY SUBROUTINES PRE                                    PRE  051
REL                                                          PRE  052
```

```
        ORG 0                                                   PRE  053
PRE     CLA D2                                                  PRE  054
        STO NG                                                  PRE  055
        TRA 1,4                                                 PRE  056
D2      PZE 0,0,2                                               PRE  057
NG      SYN 32562              77462(8) START OF COMMON         PRE  058
        END 0                                                   PRE  059

FUN     REM 1471 WRB DUMMY ROUTINES TO BE SUPERCEDED            FUN  001
        REM PROGRAM CARD 1                                      FUN  002
        FUL                                                     FUN  003
        MZE 0,0,22             9L                               FUN  004
        PZE                                                     FUN  005
        PZE D3+1                                                FUN  006
        PZE                                                     FUN  007
        BCD 1FUN1                                               FUN  008
        PZE FUN                                                 FUN  009
        BCD 1FUN2                                               FUN  010
        PZE FUN                                                 FUN  011
        BCD 1FUN3                                               FUN  012
        PZE FUN                                                 FUN  013
        BCD 1FUN4                                               FUN  014
        PZE FUN                                                 FUN  015
        BCD 1FUN5                                               FUN  016
        PZE FUN                                                 FUN  017
        BCD 1FUN6                                               FUN  018
        PZE FUN                                                 FUN  019
        BCD 1FUN7                                               FUN  020
        PZE FUN                                                 FUN  021
        BCD 1FUN8                                               FUN  022
        PZE FUN                                                 FUN  023
        BCD 1FUN9                                               FUN  024
        PZE FUN                                                 FUN  025
        BCD 1FUN10                                              FUN  026
        PZE FUN                12R                              FUN  027
        REM PROGRAM CARD 2                                      FUN  028
        MZE 0,0,20             9L                               FUN  029
        PZE                                                     FUN  030
        BCD 1FUN11                                              FUN  031
```

```
        PZE FUN                                                         FUN  032
        BCD 1FUN12                                                      FUN  033
        PZE FUN                                                         FUN  034
        BCD 1FUN13                                                      FUN  035
        PZE FUN                                                         FUN  036
        BCD 1FUN14                                                      FUN  037
        PZE FUN                                                         FUN  038
        BCD 1FUN15                                                      FUN  039
        PZE FUN                                                         FUN  040
        BCD 1FUN16                                                      FUN  041
        PZE FUN                                                         FUN  042
        BCD 1FUN17                                                      FUN  043
        PZE FUN                                                         FUN  044
        BCD 1FUN18                                                      FUN  045
        PZE FUN                                                         FUN  046
        BCD 1FUN19                                                      FUN  047
        PZE FUN                                                         FUN  048
        BCD 1FUN20                                                      FUN  049
        PZE FUN                 11R                                     FUN  050
        REM DUMMY SUBROUTINE FUN                                        FUN  051
        REL                                                             FUN  052
        ORG 0                                                           FUN  053
FUN     CLA D3                                                          FUN  054
        STO NG                                                          FUN  055
        TRA 1,4                                                         FUN  056
D3      PZE 0,0,3                                                       FUN  057
NG      SYN 32562               77462(8) START OF COMMON                FUN  058
        END 0                                                           FUN  059

OUT     REM 1471 WRB DUMMY ROUTINES TO BE SUPERCEDED                    OUT  001
        REM PROGRAM CARD 1                                              OUT  002
        FUL                                                             OUT  003
        MZE 0,0,22              9L                                      OUT  004
        PZE                                                             OUT  005
        PZE OUT+1                                                       OUT  006
        PZE                                                             OUT  007
        BCD 1OUT1                                                       OUT  008
        PZE OUT                                                         OUT  009
        BCD 1OUT2                                                       OUT  010
```

```
PZE OUT
BCD 1OUT3
PZE OUT
BCD 1OUT4
PZE OUT
BCD 1OUT5
PZE OUT
BCD 1OUT6
PZE OUT
BCD 1OUT7
PZE OUT
BCD 1OUT8
PZE OUT
BCD 1OUT9
PZE OUT
BCD 1OUT10
PZE OUT                    12R
REM PROGRAM CARD 2
MZE 0,0,20                 9L
PZE
BCD 1OUT11
PZE OUT
BCD 1OUT12
PZE OUT
BCD 1OUT13
PZE OUT
BCD 1OUT14
PZE OUT
BCD 1OUT15
PZE OUT
BCD 1OUT16
PZE OUT
BCD 1OUT17
PZE OUT
BCD 1OUT18
PZE OUT
BCD 1OUT19
PZE OUT
BCD 1OUT20
```

```
OUT  011
OUT  012
OUT  013
OUT  014
OUT  015
OUT  016
OUT  017
OUT  018
OUT  019
OUT  020
OUT  021
OUT  022
OUT  023
OUT  024
OUT  025
OUT  026
OUT  027
OUT  028
OUT  029
OUT  030
OUT  031
OUT  032
OUT  033
OUT  034
OUT  035
OUT  036
OUT  037
OUT  038
OUT  039
OUT  040
OUT  041
OUT  042
OUT  043
OUT  044
OUT  045
OUT  046
OUT  047
OUT  048
OUT  049
```

```
      PZE OUT                 11R                                          OUT  050
      REM DUMMY SUBROUTINE OUT                                             OUT  051
      REL                                                                  OUT  052
      ORG 0                                                                OUT  053
OUT   TRA 1,4                                                              OUT  054
      END 0                                                                OUT  055

CSEG2    1471 WRB SEGMENT 2 CALLING PROGRAM                                SEG2 101
      READ107                                                              SEG2 105
  107 FORMAT(72H                                                           SEG2 107
     1                 )                                                   SEG2 108
      READ505,(IC(I),I=1,10)                                               SEG2 109
      IF(IC(2))113,113,203                                                 SEG2 111
  113 CALLSUB2(P,IC)                                                       SEG2 113
      IF(IC(1)-1)117,121,125                                               SEG2 115
  117 REWIND5                                                              SEG2 117
      GOTO217                                                              SEG2 119
  121 CALLSUB3(IC(5))                                                      SEG2 121
      GOTO217                                                              SEG2 123
  125 REWIND5                                                              SEG2 125
      GOTO215                                                              SEG2 201
  203 J=IC(2)                                                              SEG2 203
      READ207,(P(I),I=1,J)                                                 SEG2 205
  207 FORMAT(8E9.4)                                                        SEG2 207
      IF(IC(1)-1)217,211,215
  211 CALLSUB20                                                            SEG2 211
      GOTO121                                                              SEG2 213
  215 CALLSUB4(IC(6))                                                      SEG2 215
  217 READ207,(A(I),I=1,6)                                                 SEG2 217
      IF(IC(3)-1)323,223,309                                               SEG2 221
  223 DO225I=1,21                                                          SEG2 223
  225 AM(I)=0.0                                                            SEG2 225
      READ207,AM(1),AM(7),AM(12),AM(16),AM(19),AM(21)                      SEG2 301
      DO305I=1,21                                                          SEG2 303
  305 AM(I)=AM(I)*AM(I)                                                    SEG2 305
      GOTO311                                                              SEG2 307
  309 READ207,(AM(I),I=1,21)                                               SEG2 309
  311 K=1                                                                  SEG2 311
      L=6                                                                  SEG2 313
```

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```
      DO321I=1,6                                                        SEG2 315
      DA(I)=(0.01)*SQRTF(AM(K))                                         SEG2 317
      K=K+L                                                             SEG2 319
  321 L=L-1                                                             SEG2 321
  323 CALLSUB5                                                          SEG2 323
      IF(IC(1))411,411,401                                              SEG2 325
  401 N=IC(5)                                                           SEG2 401
      DO407I=1,N                                                        SEG2 403
      CALLREAD(6,PM)                                                    SEG2 405
  407 DP(I)=(0.01)*SQRTF(PM(1))                                         SEG2 407
      REWIND6                                                           SEG2 409
  411 WRITEOUTPUTTAPE3,413                                              SEG2 411
  413 FORMAT(1H1)                                                       SEG2 413
      WRITEOUTPUTTAPE3,107                                              SEG2 415
      WRITEOUTPUTTAPE3,419                                              SEG2 417
  419 FORMAT(1H )                                                       SEG2 419
  421 INSAVE=IN(I)                                                      SEG2 421
  423 K=1                                                               SEG2 423
      DO509I=1,10                                                       SEG2 425
      L=K+23                                                            SEG2 501
      READ505,(IN(J),J=K,L)                                             SEG2 503
  505 FORMAT(24I3)                                                      SEG2 505
      IF(IN(L))509,511,509                                              SEG2 507
  509 K=L                                                               SEG2 509
  511 IF(IN(1))515,513,515                                              SEG2 511
  513 PAUSE77777                                                        SEG2 513
      GOTO423                                                           SEG2 514
  515 IF(IN(1)-INSAVE)517,519,517                                       SEG2 515
  517 CALLSUB7                                                          SEG2 517
  519 IF(IN(1)-100)521,521,525                                          SEG2 519
  521 CALLSUB19                                                         SEG2 521
      GOTO421                                                           SEG2 523
  525 CALLSUB21                                                         SEG2 525
      GOTO421                                                           SEG2 601
      END(0,1,0,0,0)                                                    SEG2 603

CSUB10   1471 WRB MULTIVALUED FUNCTIONS 7, 8, AND 9                     SUB10 01
      SUBROUTINESUB10                                                   SUB10 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
```

```
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      DO109I=1,3                                                         SUB10  05
      IN(4)=I                                                            SUB10  07
  109 CALLSUB19                                                          SUB10  09
      RETURN                                                             SUB10  11
      END(0,1,0,0,0)                                                     SUB10  13

CSUB5    1471 WRB READ SYMMETRY CARDS                                    SUB5  101
      SUBROUTINESUB5                                                     SUB5  103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      NS=IC(4)                                                           SUB5  105
      IF(NS-48)107,107,203                                               SUB5  201
  203 STOP5                                                              SUB5  203
  107 IF(NS)117,117,109                                                  SUB5  107
  109 DO115K=1,NS                                                        SUB5  109
      READ113,(TS(J,K),J=1,3)                                            SUB5  111
  113 FORMAT(E11.8,4H    E11.8,4H    E11.8,4H    )                       SUB5  113
  115 CALLSUB6(IS(1,1,K))                                                SUB5  115
  117 RETURN                                                             SUB5  117
      END(0,1,0,0,0)                                                     SUB5  119

CSUB8    1471 WRB COMPUTE ALL DISTANCES BETWEEN TWO MOLECULES            SUB8  101
      SUBROUTINESUB8                                                     SUB8  103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      IF(IN(6))107,107,111                                               SUB8  105
  107 DMAX=4.0                                                           SUB8  107
      GOTO113                                                            SUB8  109
  111 DMAX=IN(6)/10                                                      SUB8  111
  113 N=IN(2)                                                            SUB8  113
      IF(N)217,217,117                                                   SUB8  115
  117 DO215I=1,N                                                         SUB8  117
      IN(2)=I                                                            SUB8  119
      DO213J=1,N                                                         SUB8  121
      IF(IN(3)-IN(5))201,125,201                                         SUB8  123
```

```
  125 IF(J-I)201,215,215                                                SUB8 125
  201 IN(4)=J                                                           SUB8 201
      NG=0                                                              SUB8 203
      CALLSUB12                                                         SUB8 205
      IF(FX-DMAX)209,209,213                                            SUB8 207
  209 F=FX                                                              SUB8 209
      CALLSUB13                                                         SUB8 211
  213 CONTINUE                                                          SUB8 213
  215 CONTINUE                                                          SUB8 215
  217 RETURN                                                            SUB8 217
      END(0,1,0,0,0)                                                    SUB8 219

CSUB11   1471 WRB MULTIVALUED FUNCTIONS 10 AND 11                       SUB11 01
      SUBROUTINESUB11                                                   SUB11 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DO113I=1,3                                                        SUB11 05
      IN(4)=I                                                           SUB11 07
      DO113J=1,3                                                        SUB11 09
      IN(5)=J                                                           SUB11 11
  113 CALLSUB19                                                         SUB11 13
      RETURN                                                            SUB11 15
      END(0,1,0,0,0)                                                    SUB11 17

CSUB13   1471 WRB ERROR CALCULATION AND OUTPUT                          SUB13101
      SUBROUTINESUB13
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      IF(NG)105,113,105                                                 SUB13103
  105 WRITEOUTPUTTAPE3,107,NG                                           SUB13105
  107 FORMAT(55H0                                                   *** SUB13107
     1I3)                                                               SUB13109
      GOTO715                                                           SUB13111
  113 VARA=0.0                                                          SUB13113
      VARP=0.0                                                          SUB13115
      IF(IC(3))119,313,119                                              SUB13117
  119 DO211I=1,6                                                        SUB13120
```

```
      IF(DA(I))201,123,201                                              SUB13121
  123 DFDA(I)=0.0                                                       SUB13123
      GOTO211                                                           SUB13125
  201 SAVEA=A(I)                                                        SUB13201
      A(I)=A(I)+DA(I)                                                   SUB13203
      CALLSUB12                                                         SUB13205
      A(I)=SAVEA                                                        SUB13207
      DFDA(I)=(FX-F)/DA(I)                                              SUB13209
  211 CONTINUE                                                          SUB13211
      K=1                                                               SUB13213
      L=6                                                               SUB13215
      DO311I=1,6                                                        SUB13217
      IF(DFDA(I))225,221,225                                            SUB13219
  221 K=K+L                                                             SUB13221
      GOTO311                                                           SUB13223
  225 C=1.0                                                             SUB13225
      DO309J=I,6                                                        SUB13301
      IF(DFDA(J))305,307,305                                            SUB13303
  305 VARA=VARA+C*DFDA(I)*DFDA(J)*AM(K)                                 SUB13305
  307 K=K+1                                                             SUB13307
  309 C=2.0                                                             SUB13309
  311 L=L-1                                                             SUB13311
  313 IF(IC(1))315,525,315                                              SUB13313
  315 CALLSUB14                                                         SUB13315
      CALLSUB16                                                         SUB13317
      J=0                                                               SUB13319
      N=IC(5)                                                           SUB13321
      DO423I=1,N                                                        SUB13323
  325 J=J+1                                                             SUB13325
      S=SUB17(J)                                                        SUB13401
  403 IF(S)407,325,411                                                  SUB13403
      FREQUENCY403(10,2,1)                                              SUB13405
  407 DFDP(I)=0.0                                                       SUB13407
      GOTO423                                                           SUB13409
  411 IF(DP(I))413,407,413                                              SUB13411
  413 SAVEP=P(J)                                                        SUB13413
      P(J)=P(J)+DP(I)                                                   SUB13415
      CALLSUB12                                                         SUB13417
      P(J)=SAVEP                                                        SUB13419
```

```
      DFDP(I)=(FX-F)/DP(I)                                      SUB13421
      L=I                                                       SUB13422
  423 CONTINUE                                                  SUB13423
      DO519I=1,L                                                SUB13425
      CALLREAD(6,PM)                                            SUB13501
  503 IF(DFDP(I))505,519,505                                    SUB13503
  505 C=1.0                                                     SUB13505
      K=1                                                       SUB13507
      DO517J=I,L                                                SUB13509
  511 IF(DFDP(J))513,515,513                                    SUB13511
  513 VARP=VARP+C*DFDP(I)*DFDP(J)*PM(K)                         SUB13513
  515 K=K+1                                                     SUB13515
  517 C=2.0                                                     SUB13517
  519 CONTINUE                                                  SUB13519
      FREQUENCY503(1,10,1),511(1,10,1)                          SUB13521
      REWIND6                                                   SUB13523
  525 IF(NG)601,609,601                                         SUB13525
  601 WRITEOUTPUTTAPE3,603,F,NG                                 SUB13601
  603 FORMAT(49H0                                        F9.4,  SUB13603
     19H       ***I3)                                           SUB13605
      GOTO715                                                   SUB13607
  609 E1=SQRTF(VARP)                                            SUB13609
      E=SQRTF(VARP+VARA)                                        SUB13611
      IF(IC(1))615,617,615                                      SUB13613
  615 IF(IC(3))619,701,619                                      SUB13615
  617 IF(IC(3))701,709,701                                      SUB13617
  619 WRITEOUTPUTTAPE3,621,F,E,E1                               SUB13619
  621 FORMAT(49H0                                               SUB13621
     1F9.4,5H +OR-F7.4,2H (F7.4,1H))                            SUB13623
      GOTO715                                                   SUB13625
  701 WRITEOUTPUTTAPE3,703,F,E                                  SUB13701
  703 FORMAT(49H0                                               SUB13703
     1F9.4,5H +OR-F7.4)                                         SUB13705
      GOTO715                                                   SUB13707
  709 WRITE OUTPUT TAPE 3, 711, F                               SUB13709
  711 FORMAT(49H0                                        F9.4)  SUB13711
  715 CALLSUB18                                                 SUB13715
      RETURN                                                    SUB13717
      END(0,1,0,0,0)                                            SUB13719
```

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CSUB19   1471 WRB FUNCTION AND ERROR CALCULATION                          SUB19101
      SUBROUTINESUB19                                                     SUB19103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P           COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)      DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)    DIM   03
      NG=0                                                                SUB19105
      IF(IN(1))117,117,109                                                SUB19107
  109 IF(IN(1)-20)111,111,117                                             SUB19109
  111 CALLSUB12                                                           SUB19111
      F=FX                                                                SUB19113
      CALLSUB13                                                           SUB19115
  117 RETURN                                                              SUB19117
      END(0,1,0,0,0)                                                      SUB19119

CSUB21   1471 WRB COMPUTE MULTIVALUED FUNCTIONS                           SUB21101
      SUBROUTINESUB21                                                     SUB21103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P           COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)      DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)    DIM   03
      IH=IN(1)/100                                                        SUB21105
      IN(1)=IN(1)-100*IH                                                  SUB21107
      IF(IN(1)-11)111,111,319                                             SUB21109
  111 IF(IN(1)-9)113,113,305                                              SUB21111
  113 IF(IN(1)-6)115,115,215                                              SUB21113
  115 IF(IN(1)-1)117,117,319                                              SUB21115
  117 IF(IH-1)119,119,123                                                 SUB21117
  119 CALLSUB8                                                            SUB21119
      GOTO319                                                             SUB21121
  123 N=IN(2)                                                             SUB21123
      M=IC(4)+1                                                           SUB21125
      IN(3)=0                                                             SUB21201
      DO211I=1,8                                                          SUB21203
      DO211J=1,M                                                          SUB21205
      IN(2)=N                                                             SUB21207
      IN(5)=100*(I-1)+J-1                                                 SUB21209
  211 CALLSUB8                                                            SUB21211
      GOTO319                                                             SUB21213
  215 IF(IH-1)217,217,221                                                 SUB21215
```

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  217 CALLSUB10                                                          SUB21217
      GOTO319                                                            SUB21219
  221 N=IN(2)                                                            SUB21221
      DO301I=1,N                                                         SUB21223
      IN(2)=I                                                            SUB21225
  301 CALLSUB10                                                          SUB21301
      GOTO319                                                            SUB21303
  305 IF(IH-1)307,307,311                                                SUB21305
  307 CALLSUB11                                                          SUB21307
      GOTO319                                                            SUB21309
  311 N=IN(2)                                                            SUB21311
      DO317I=1,N                                                         SUB21313
      IN(2)=I                                                            SUB21315
  317 CALLSUB11                                                          SUB21317
  319 RETURN                                                             SUB21319
      END(0,1,0,0,0)                                                     SUB21321

CSETKX   1471 WRB SET KEY WORDS FOR ATOM COORDINATES                     SETKX1
      SUBROUTINESETKX(I)                                                 SETKX1
C     I=IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER        SETKX1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM   03
      DIMENSIONK3(3)                                                     SETKX1
      IF(I)123,123,111                                                   SETKX1
  111 K3(1)=3                                                            SETKX1
      J=IC(8)+IC(7)*(I-1)                                                SETKX1
      K=J/36                                                             SETKX1
      K3(2)=J-36*K                                                       SETKX1
      K3(3)=K+1                                                          SETKX1
      CALLSUB15(K3)                                                      SETKX1
  123 RETURN                                                             SETKX1
      END(0,1,0,0,0)                                                     SETKX1

CSETKB   1471 WRB SET KEY WORDS FOR ATOM BETAS                           SETKB1
      SUBROUTINESETKB(I)                                                 SETKB1
C     I=IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER        SETKB1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM   01
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      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONK3(3)                                                     SETKB1
      IF(I)123,123,111                                                   SETKB1
  111 K3(1)=6                                                            SETKB1
      J=IC(10)+IC(9)*(I-1)                                               SETKB1
      K=J/36                                                             SETKB1
      K3(2)=J-36*K                                                       SETKB1
      K3(3)=K+1                                                          SETKB1
      CALLSUB15(K3)                                                      SETKB1
  123 RETURN                                                             SETKB1
      END(0,1,0,0,0)                                                     SETKB1

CSTOAA   1471 WRB STORE METRIC TENSOR                                    STOAA1
      SUBROUTINESTOAA                                                    STOAA1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      AA(1,1)=A(1)*A(1)                                                  STOAA1
      AA(2,2)=A(2)*A(2)                                                  STOAA1
      AA(3,3)=A(3)*A(3)                                                  STOAA1
      AA(1,2)=A(1)*A(2)*A(6)                                             STOAA1
      AA(2,1)=AA(1,2)                                                    STOAA1
      AA(1,3)=A(1)*A(3)*A(5)                                             STOAA1
      AA(3,1)=AA(1,3)                                                    STOAA1
      AA(2,3)=A(2)*A(3)*A(4)                                             STOAA1
      AA(3,2)=AA(2,3)                                                    STOAA1
      RETURN                                                             STOAA1
      END(0,1,0,0,0)                                                     STOAA1

CSTOBB   1471 WRB STORE RECIPROCAL METRIC TENSOR                         STOBB101
      SUBROUTINESTOBB                                                    STOBB103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONAI(6),CI(6),BBII(3),BBJK(3)                               STOBB105
      DO121I=1,3                                                         STOBB107
      IF(A(I))111,111,115                                                STOBB109
  111 NG=6                                                               STOBB111
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```
      GOTO225                                                           STOBB113
  115 AI(I)=A(I)                                                        STOBB115
      AI(I+3)=A(I)                                                      STOBB117
      CI(I)=A(I+3)                                                      STOBB119
  121 CI(I+3)=A(I+3)                                                    STOBB121
      X=1.0/(AI(1)*AI(2)*AI(3)*(1.0-CI(1)*CI(1)-CI(2)*CI(2)             STOBB123
     1-CI(3)*CI(3)+2.0*CI(1)*CI(2)*CI(3)))                              STOBB125
      DO205I=1,3                                                        STOBB201
      BBII(I)=X*(1.0-CI(I)*CI(I))*AI(I+1)*AI(I+2)/AI(I)                 STOBB203
  205 BBJK(I)=X*AI(I)*(CI(I+1)*CI(I+2)-CI(I))                           STOBB205
      BB(1,1)=BBII(1)                                                   STOBB207
      BB(1,2)=BBJK(3)                                                   STOBB209
      BB(1,3)=BBJK(2)                                                   STOBB211
      BB(2,1)=BBJK(3)                                                   STOBB213
      BB(2,2)=BBII(2)                                                   STOBB215
      BB(2,3)=BBJK(1)                                                   STOBB217
      BB(3,1)=BBJK(2)                                                   STOBB219
      BB(3,2)=BBJK(1)                                                   STOBB221
      BB(3,3)=BBII(3)                                                   STOBB223
  225 RETURN                                                            STOBB225
      END(0,1,0,0,0)                                                    STOBB227

CATOM    1471 WRB ATOM COORDINATE SUBROUTINE                            ATOM 101
      SUBROUTINEATOM(I,Z)                                               ATOM 103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONI(2),X(3),Y(3),Z(3)                                      ATOM 105
      IF(I(1))109,109,117                                               ATOM 107
  109 X(1)=0.0                                                          ATOM 109
      X(2)=0.0                                                          ATOM 111
      X(3)=0.0                                                          ATOM 113
      GOTO125                                                           ATOM 115
  117 K=IC(7)*(I(1)-1)+IC(8)                                            ATOM 117
      IF(K+2-IC(2))119,119,503                                          ATOM 501
  503 NG=5                                                              ATOM 503
      GOTO325                                                           ATOM 505
  119 DO123J=1,3                                                        ATOM 119
      X(J)=P(K)                                                         ATOM 121
```

```
  123 K=K+1                                                          ATOM 123
  125 KC=I(2)/100                                                    ATOM 125
      KS=I(2)-100*KC                                                 ATOM 201
      IF(KS-IC(4))203,203,403                                        ATOM 401
  403 NG=1                                                           ATOM 403
      GOTO325                                                        ATOM 405
  203 IF(KS)403,205,213                                              ATOM 203
  205 Y(1)=X(1)                                                      ATOM 205
      Y(2)=X(2)                                                      ATOM 207
      Y(3)=X(3)                                                      ATOM 209
      GOTO311                                                        ATOM 211
  213 DO215J=1,3                                                     ATOM 213
  215 Y(J)=TS(J,KS)                                                  ATOM 215
      DO309K=1,3                                                     ATOM 217
      DO307J=1,2                                                     ATOM 219
      L=IS(J,K,KS)                                                   ATOM 221
      IF(L)225,307,305                                               ATOM 223
  225 L=-L                                                           ATOM 225
      Y(K)=Y(K)-X(L)                                                 ATOM 301
      GOTO307                                                        ATOM 303
  305 Y(K)=Y(K)+X(L)                                                 ATOM 305
  307 CONTINUE                                                       ATOM 307
  309 CONTINUE                                                       ATOM 309
  311 KC4=KC/4                                                       ATOM 311
      KC3=KC-4*KC4                                                   ATOM 313
      KC2=KC3/2                                                      ATOM 315
      KC1=KC3-2*KC2                                                  ATOM 317
      Z(1)=Y(1)-FLOATF(KC1)                                          ATOM 319
      Z(2)=Y(2)-FLOATF(KC2)                                          ATOM 321
      Z(3)=Y(3)-FLOATF(KC4)                                          ATOM 323
  325 RETURN                                                         ATOM 325
      END(0,1,0,0,0)                                                 ATOM 327

CBETA    1471 WRB STORE TRANSFORMED ANISOTROPIC TEMP FACTOR MATRIX   BETA 1
      SUBROUTINEBETA(INS,Z)                                          BETA 1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P      COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6) DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300) DIM   03
      DIMENSIONINS(2),Z(3,3),B1(6),B2(9)                             BETA 1
```

```
C     INS IS ATOM DESCRIPTION, Z IS TRANSFORMED MATRIX                  BETA 1
      IF(IC(9)-6)111,115,115                                            BETA 1
  111 NG=4                                                              BETA 1
      GOTO423                                                           BETA 1
  115 KS=XMODF(INS(2),100)                                              BETA 1
      IF(KS)121,119,119                                                 BETA 1
  119 IF(KS-IC(4))125,125,121                                           BETA 1
  121 NG=1                                                              BETA 1
      GOTO423                                                           BETA 1
  125 IF(INS(1))211,201,207                                             BETA 1
  201 DO203I=1,6                                                        BETA 2
  203 B1(I)=0.0                                                         BETA 2
      GOTO221                                                           BETA 2
  207 J=IC(10)+IC(9)*(INS(1)-1)                                         BETA 2
      IF(J+5-IC(2))215,215,211                                          BETA 2
  211 NG=5                                                              BETA 2
      GOTO423                                                           BETA 2
  215 DO219I=1,6                                                        BETA 2
      B1(I)=P(J)                                                        BETA 2
  219 J=J+1                                                             BETA 2
  221 B2(1)=B1(1)                                                       BETA 2
      B2(2)=B1(4)                                                       BETA 2
      B2(3)=B1(5)                                                       BETA 2
      B2(4)=B1(2)                                                       BETA 3
      B2(6)=B1(6)                                                       BETA 3
      B2(9)=B1(3)                                                       BETA 3
      DO421I=1,3                                                        BETA 3
      DO419J=I,3                                                        BETA 3
      IF(KS)121,313,319                                                 BETA 3
  313 M=I*J                                                             BETA 3
      B3=B2(M)                                                          BETA 3
      GOTO415                                                           BETA 3
  319 B3=0.0                                                            BETA 3
      DO413K=1,2                                                        BETA 3
      DO411L=1,2                                                        BETA 3
      M=IS(K,I,KS)*IS(L,J,KS)                                           BETA 3
      IF(M)407,411,403                                                  BETA 4
  403 B3=B3+B2(M)                                                       BETA 4
      GOTO411                                                           BETA 4
```

```
  407 M=-M                                                          BETA 4
      B3=B3-B2(M)                                                   BETA 4
  411 CONTINUE                                                      BETA 4
  413 CONTINUE                                                      BETA 4
  415 Z(I,J)=B3                                                     BETA 4
      Z(J,I)=B3                                                     BETA 4
  419 CONTINUE                                                      BETA 4
  421 CONTINUE                                                      BETA 4
  423 RETURN                                                        BETA 4
      END(0,1,0,0,0)                                                BETA 4

CMM       1471 WRB MULTIPLY TWO MATRICES                            MM   101
C                  Z(3,3)=X(3,3)*Y(3,3)                             MM   103
      SUBROUTINEMM(X,Y,Z)                                           MM   105
      DIMENSIONX(3,3),Y(3,3),Z(3,3)                                 MM   107
      DO117I=1,3                                                    MM   109
      DO117K=1,3                                                    MM   111
      Z(I,K)=0.0                                                    MM   113
      DO117J=1,3                                                    MM   115
  117 Z(I,K)=Z(I,K)+X(I,J)*Y(J,K)                                   MM   117
      RETURN                                                        MM   119
      END(0,1,0,0,0)                                                MM   121

CMV       1471 WRB MATRIX * VECTOR                                  MV   1
C                  Z(3)=X(3,3)*Y(3)                                 MV   1
      SUBROUTINEMV(X,Y,Z)                                           MV   1
      DIMENSIONX(3,3),Y(3),Z(3)                                     MV   1
      DO113I=1,3                                                    MV   1
      Z(I)=0.0                                                      MV   1
      DO113J=1,3                                                    MV   1
  113 Z(I)=Z(I)+X(I,J)*Y(J)                                         MV   1
      RETURN                                                        MV   1
      END(0,1,0,0,0)                                                MV   1

CVM       1471 WRB TRANSPOSED VECTOR TIMES MATRIX                   VM   101
C                  Z(3)=X(3)*Y(3,3)                                 VM   103
      SUBROUTINEVM(X,Y,Z)                                           VM   105
      DIMENSIONX(3),Y(3,3),Z(3)                                     VM   107
      DO115J=1,3                                                    VM   109
```

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```
      Z(J)=0.0                                                          VM    111
      DO115I=1,3                                                        VM    113
  115 Z(J)=Z(J)+X(I)*Y(I,J)                                             VM    115
      RETURN                                                            VM    117
      END(0,1,0,0,0)                                                    VM    119

CVV       1471 WRB TRANSPOSED VECTOR * VECTOR                           VV    1
C                  VV=X(3)*Y(3)                                         VV    1
      FUNCTIONVV(X,Y)                                                   VV    1
      DIMENSIONX(3),Y(3)                                                VV    1
      VV=0.0                                                            VV    1
      DO111I=1,3                                                        VV    1
  111 VV=VV+X(I)*Y(I)                                                   VV    1
      RETURN                                                            VV    1
      END(0,1,0,0,0)                                                    VV    1

CVMV      1471 WRB TRANSPOSED VECTOR * MATRIX * VECTOR                  VMV   1
C                  VMV=W(3)*X(3,3)*Y(3)                                 VMV   1
      FUNCTIONVMV(W,X,Y)                                                VMV   1
      DIMENSIONW(3),X(3,3),Y(3),Z(3)                                    VMV   1
      CALLMV(X,Y,Z)                                                     VMV   1
      VMV=VV(W,Z)                                                       VMV   1
      RETURN                                                            VMV   1
      END(0,1,0,0,0)                                                    VMV   1

CDIFV     1471 WRB VECTOR - VECTOR                                      DIFV  1
C                  Z(3)=X(3)-Y(3)                                       DIFV  1
      SUBROUTINEDIFV(X,Y,Z)                                             DIFV  1
      DIMENSIONX(3),Y(3),Z(3)                                           DIFV  1
      DO111I=1,3                                                        DIFV  1
  111 Z(I)=X(I)-Y(I)                                                    DIFV  1
      RETURN                                                            DIFV  1
      END(0,1,0,0,0)                                                    DIFV  1

CSUMV     1471 WRB COMPUTE THE SUM OF TWO VECTORS                       SUMV  101
C                  Z(3)=X(3)+Y(3)                                       SUMV  103
      SUBROUTINESUMV(X,Y,Z)                                             SUMV  105
      DIMENSIONX(3),Y(3),Z(3)                                           SUMV  107
      DO111I=1,3                                                        SUMV  109
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  111 Z(I)=X(I)+Y(I)
      RETURN                                                            SUMV 111
      END(0,1,0,0,0)                                                    SUMV 113
                                                                        SUMV 115
CCOSVV   1471 WRB COSINE OF ANGLE BETWEEN VECTORS X AND Y
      FUNCTIONCOSVV(X,Y)                                                COSVV101
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COSVV103
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    COM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   01
      DIMENSIONX(3),Y(3)                                                DIM   03
      D=SQRTF(VMV(X,AA,X)*VMV(Y,AA,Y))                                  COSVV105
      IF(D)111,111,115                                                  COSVV107
  111 NG=9                                                              COSVV109
      GOTO117                                                           COSVV111
  115 COSVV=VMV(X,AA,Y)/D                                               COSVV113
  117 RETURN                                                            COSVV115
      END(0,1,0,0,0)                                                    COSVV117
                                                                        COSVV119
CARCCOS  1471 WRB ARCCOS(X) IN DEGREES
      FUNCTIONARCCOS(X)                                                 ARCCOS01
      ARCCOS=90.0-(57.29577951)*SIGNF(ASINF(X),X)                       ARCCOS03
      RETURN                                                            ARCCOS05
      END(0,1,0,0,0)                                                    ARCCOS07
                                                                        ARCCOS09
CNORM    1471 WRB STORE A VECTOR Z NORMAL TO VECTORS X AND Y
      SUBROUTINENORM(X,Y,Z)                                             NORM 101
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         NORM 103
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    COM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   01
      DIMENSIONX(3),Y(3),Z(3),X1(6),Y1(6),Z1(3)                         DIM   03
      DO115I=1,3                                                        NORM 105
      X1(I)=X(I)                                                        NORM 107
      X1(I+3)=X(I)                                                      NORM 109
      Y1(I)=Y(I)                                                        NORM 111
  115 Y1(I+3)=Y(I)                                                      NORM 113
      DO119I=1,3                                                        NORM 115
  119 Z1(I)=X1(I+1)*Y1(I+2)-X1(I+2)*Y1(I+1)                             NORM 117
      CALLMV(BB,Z1,Z)                                                   NORM 119
      RETURN                                                            NORM 121
                                                                        NORM 123
```

```
      END(0,1,0,0,0)                                                    NORM 125

CAXES    1471 WRB STORE THREE MUTUALLY PERPENDICULAR                    AXES 101
C                 VECTORS X(I,1), X(I,2), AND X(I,3) GIVEN              AXES 103
C                 VECTORS U AND V.                                      AXES 105
      SUBROUTINEAXES(U,V,X)                                             AXES 107
      DIMENSIONU(3),V(3),X(3,3)                                         AXES 109
      DO113I=1,3                                                        AXES 111
  113 X(I,1)=U(I)                                                       AXES 113
      CALLNORM(U,V,X(1,2))                                              AXES 115
      CALLNORM(X(1,1),X(1,2),X(1,3))                                    AXES 117
      RETURN                                                            AXES 119
      END(0,1,0,0,0)                                                    AXES 121

CEIGVAL  1471 WRB FIND EIGENVALUES Y OF MATRIX W                        EIGVAL01
      SUBROUTINEEIGVAL(W,Y)                                             EIGVAL03
      COMMONNG                                                          EIGVAL04
      DIMENSIONW(3,3),Y(3),X(3),Z(6,6)                                  EIGVAL05
      DO119J=1,3                                                        EIGVAL07
      DO119I=1,3                                                        EIGVAL09
      Z1=W(I,J)                                                         EIGVAL11
      Z(I,J)=Z1                                                         EIGVAL13
      Z(I+3,J)=Z1                                                       EIGVAL15
      Z(I,J+3)=Z1                                                       EIGVAL17
  119 Z(I+3,J+3)=Z1                                                     EIGVAL19
      P=0.0                                                             EIGVAL21
      Q=0.0                                                             EIGVAL23
      R=0.0                                                             EIGVAL25
      DO207I=1,3                                                        EIGVAL01
      P=P-Z(I,I)                                                        EIGVAL03
      Q=Q+Z(I,I)*Z(I+1,I+1)-Z(I,I+1)*Z(I+1,I)                           EIGVAL05
  207 R=R+Z(3,I)*Z(2,I+1)*Z(1,I+2)-Z(1,I)*Z(2,I+1)*Z(3,I+2)             EIGVAL07
      P3=P/3.0                                                          EIGVAL09
      A=Q-P*P3                                                          EIGVAL11
      B=2.0*P3*P3*P3-Q*P3+R                                             EIGVAL13
      B2=B/2.0                                                          EIGVAL15
      A3=A/3.0                                                          EIGVAL17
      B4=B2*B2                                                          EIGVAL19
      A27=A3*A3*A3                                                      EIGVAL21
```

```
      IF(B4+A27)303,303,225                                          EIGVAL23
  225 NG=7                                                           EIGVAL25
      GOTO317                                                        EIGVAL01
  303 PHI3=(ASINF(SQRTF(1.0+(B4/A27))))/3.0                          EIGVAL03
      C=-SIGNF((2.0*SQRTF(-A3)),B)                                   EIGVAL05
      X(1)=C*COSF(PHI3)                                              EIGVAL07
      X(2)=C*COSF(PHI3+4.188790205)                                  EIGVAL09
      X(3)=C*COSF(PHI3+2.094395103)                                  EIGVAL11
      DO315I=1,3                                                     EIGVAL13
  315 Y(I)=X(I)-P3                                                   EIGVAL15
  317 RETURN                                                         EIGVAL17
      END(0,1,0,0,0)                                                 EIGVAL19

CEIGVEC  1471 WRB COMPUTE EIGENVECTOR Z OF MATRIX                    EIGVEC01
C                 W GIVEN EIGENVALUE Y                               EIGVEC03
      SUBROUTINEEIGVEC(W,Y,Z)                                        EIGVEC05
      COMMONNG                                                       EIGVEC07
      DIMENSIONW(3,3),X(6,6),Z(3),P(3)                               EIGVEC09
      DO123J=1,3                                                     EIGVEC11
      DO123I=1,3                                                     EIGVEC13
      X1=W(I,J)                                                      EIGVEC15
      X(I,J)=X1                                                      EIGVEC17
      X(I+3,J)=X1                                                    EIGVEC19
      X(I,J+3)=X1                                                    EIGVEC21
  123 X(I+3,J+3)=X1                                                  EIGVEC23
      Y1=Y                                                           EIGVEC25
      DO209I=1,3                                                     EIGVEC01
      X(I,I)=X(I,I)-Y1                                               EIGVEC03
      X(I+3,I)=X(I+3,I)-Y1                                           EIGVEC05
      X(I,I+3)=X(I,I+3)-Y1                                           EIGVEC07
  209 X(I+3,I+3)=X(I+3,I+3)-Y1                                       EIGVEC09
      S1=0.0                                                         EIGVEC11
      DO307I=1,3                                                     EIGVEC13
      S=0.0                                                          EIGVEC15
      DO223J=1,3                                                     EIGVEC17
      PJ=X(I,J+1)*X(I+1,J+2)-X(I,J+2)*X(I+1,J+1)                     EIGVEC01
      P(J)=PJ                                                        EIGVEC21
  223 S=S+PJ*PJ                                                      EIGVEC23
      IF(S-S1)307,307,301                                            EIGVEC25
```

```
  301 S1=S                                                              EIGVEC01
      DO305J=1,3                                                        EIGVEC03
  305 Z(J)=P(J)                                                         EIGVEC05
  307 CONTINUE                                                          EIGVEC07
      IF(S1)311,311,313                                                 EIGVEC09
  311 NG=8                                                              EIGVEC11
  313 RETURN                                                            EIGVEC13
      END(0,1,0,0,0)                                                    EIGVEC15

CTRACE   1471 WRB COMPUTE TRACE OF MATRIX X                             TRACE101
      FUNCTIONTRACE(X)                                                  TRACE103
      DIMENSIONX(3,3)                                                   TRACE105
      TRACE=0.0                                                         TRACE107
      DO111I=1,3                                                        TRACE109
  111 TRACE=TRACE+X(I,I)                                                TRACE111
      RETURN                                                            TRACE113
      END(0,1,0,0,0)                                                    TRACE115

CFUNA    1471 WRB ANGLE SUBROUTINE USED BY FUN2, FUN5, FUN6             FUNA  01
      FUNCTIONFUNA(I)                                                   FUNA  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONI(6),X1(3),X2(3),X3(3),V1(3),V2(3)                       FUNA  05
      CALLSTOAA                                                         FUNA  07
      CALLATOM(I(1),X1)                                                 FUNA  09
      CALLATOM(I(3),X2)                                                 FUNA  11
      CALLATOM(I(5),X3)                                                 FUNA  13
      IF(NG)123,117,123                                                 FUNA  15
  117 CALLDIFV(X1,X2,V1)                                                FUNA  17
      CALLDIFV(X3,X2,V2)                                                FUNA  19
      FUNA=ARCCOS(COSVV(V1,V2))                                         FUNA  21
  123 RETURN                                                            FUNA  23
      END(0,1,0,0,0)                                                    FUNA  25

CFUND    1471 WRB DISTANCE SUBROUTINE USED BY FUN1 AND FUN4             FUND  01
      FUNCTIONFUND(I)                                                   FUND  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
```

```
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONI(4),X1(3),X2(3),V(3)                                    FUND  05
      CALLSTOAA                                                         FUND  07
      CALLATOM(I(1),X1)                                                 FUND  09
      CALLATOM(I(3),X2)                                                 FUND  11
      CALLDIFV(X2,X1,V)                                                 FUND  13
      FUND=SQRTF(VMV(V,AA,V))                                           FUND  15
      RETURN                                                            FUND  17
      END(0,1,0,0,0)                                                    FUND  19

CHED1    1471 WRB HEADING 1                                             HED1  01
      SUBROUTINEHED1                                                    HED1  03
      WRITEOUTPUTTAPE3,107                                              HED1  05
  107 FORMAT(34H0INTERATOMIC DISTANCE IN ANGSTROMS)                     HED1 107
      RETURN                                                            HED1  09
      END(0,1,0,0,0)                                                    HED1  11

CPRE1    1471 WRB SET KEY WORDS FOR INTERATOMIC DISTANCE                PRE1 1
      SUBROUTINEPRE1                                                    PRE1 1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      CALLSETKX(IN(2))                                                  PRE1 1
      CALLSETKX(IN(4))                                                  PRE1 1
      RETURN                                                            PRE1 1
      END(0,1,0,0,0)                                                    PRE1 1

CFUN1    1471 WRB COMPUTE INTERATOMIC DISTANCE                          FUN1  01
      SUBROUTINEFUN1                                                    FUN1  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      FX=FUND(IN(2))                                                    FUN1  05
      RETURN                                                            FUN1  07
      END(0,1,0,0,0)                                                    FUN1  09

COUT1    1471 WRB PUT OUT DESCRIPTION OF INTERATOMIC DISTANCE           OUT1 1
      SUBROUTINEOUT1                                                    OUT1 1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
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      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,5)                                 OUT1  1
  107 FORMAT(12H+          (I2,1H,I3,3H) (I2,1H,I3,1H))                  OUT1  1
      RETURN                                                             OUT1  1
      END(0,1,0,0,0)                                                     OUT1  1

CHED2    1471 WRB HEADING 2                                              HED2   01
      SUBROUTINEHED2                                                     HED2   03
      WRITEOUTPUTTAPE3,107                                               HED2   05
  107 FORMAT(46H0BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX)          HED2  107
      RETURN                                                             HED2   09
      END(0,1,0,0,0)                                                     HED2   11

CPRE2    1471 WRB PRELIMINARY SUBROUTINE 2                               PRE2   01
      SUBROUTINEPRE2                                                     PRE2   03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      DO107I=2,6,2                                                       PRE2   05
  107 CALLSETKX(IN(I))                                                   PRE2   07
      RETURN                                                             PRE2   09
      END(0,1,0,0,0)                                                     PRE2   11

CFUN2    1471 WRB BOND ANGLE SUBROUTINE                                  FUN2   01
      SUBROUTINEFUN2                                                     FUN2   03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      FX=FUNA(IN(2))                                                     FUN2   05
      RETURN                                                             FUN2   07
      END(0,1,0,0,0)                                                     FUN2   09

COUT2    1471 WRB OUTPUT DESCRIPTION 2                                   OUT2   01
      SUBROUTINEOUT2                                                     OUT2   03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,7)                                 OUT2   05
```

```
  107 FORMAT(12H+          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H))   OUT2 107
      RETURN                                                            OUT2  09
      END(0,1,0,0,0)                                                    OUT2  11

CHED3    1471 WRB HEADING 3                                             HED3  01
      SUBROUTINEHED3                                                    HED3  03
      WRITEOUTPUTTAPE3,107                                              HED3  05
  107 FORMAT(58H0DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOHED3 107
     1MS)                                                               HED3 108
      RETURN                                                            HED3  09
      END(0,1,0,0,0)                                                    HED3  11

CPRE3    1471 WRB PRELIMINARY SUBROUTINE 3                              PRE3  01
      SUBROUTINEPRE3                                                    PRE3  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DO107I=2,12,2                                                     PRE3  05
  107 CALLSETKX(IN(I))                                                  PRE3  07
      RETURN                                                            PRE3  09
      END(0,1,0,0,0)                                                    PRE3  11

CFUN3    1471 WRB DIHEDRAL ANGLE SUBROUTINE                             FUN3  01
      SUBROUTINEFUN3                                                    FUN3  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONX(3,6),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3)               FUN3  05
      CALLSTOAA                                                         FUN3  07
      CALLSTOBB                                                         FUN3  09
      IF(NG)207,113,207                                                 FUN3  11
  113 DO115I=1,6                                                        FUN3  13
  115 CALLATOM(IN(2*I),X(1,I))                                          FUN3  15
      IF(NG)207,119,207                                                 FUN3  17
  119 CALLDIFV(X(1,2),X(1,1),V1)                                        FUN3  19
      CALLDIFV(X(1,3),X(1,1),V2)                                        FUN3  21
      CALLDIFV(X(1,5),X(1,4),V3)                                        FUN3  23
      CALLDIFV(X(1,6),X(1,4),V4)                                        FUN3  25
      CALLNORM(V1,V2,V5)                                                FUN3  01
```

```
      CALLNORM(V3,V4,V6)                                                FUN3  03
      FX=ARCCOS(COSVV(V5,V6))                                           FUN3  05
  207 RETURN                                                            FUN3  07
      END(0,1,0,0,0)                                                    FUN3  09

COUT3    1471 WRB OUTPUT DESCRIPTION 3                                  OUT3  01
      SUBROUTINEOUT3                                                    OUT3  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,13)                               OUT3  05
  107 FORMAT(12H+          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)/12HOUT3 107
     1           (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H))             OUT3 108
      RETURN                                                            OUT3  09
      END(0,1,0,0,0)                                                    OUT3  11

CHED4    1471 WRB HEADING 4                                             HED4  01
      SUBROUTINEHED4                                                    HED4  03
      WRITEOUTPUTTAPE3,107                                              HED4  05
  107 FORMAT(45H0DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES)          HED4 107
      RETURN                                                            HED4  11
      END(0,1,0,0,0)                                                    HED4  13

CPRE4    1471 WRB PRELIMINARY SUBROUTINE 4                              PRE4  01
      SUBROUTINEPRE4                                                    PRE4  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DO107I=2,8,2                                                      PRE4  05
  107 CALLSETKX(IN(I))                                                  PRE4  07
      RETURN                                                            PRE4  09
      END(0,1,0,0,0)                                                    PRE4  11

CFUN4    1471 WRB DIFFERENCE BETWEEN BOND DISTANCES                     FUN4  01
      SUBROUTINEFUN4                                                    FUN4  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      FX=FUND(IN(2))-FUND(IN(6))                                        FUN4  05
```

```
      RETURN                                                            FUN4  07
      END(0,1,0,0,0)                                                    FUN4  09

COUT4    1471 WRB OUTPUT DESCRIPTION 4                                  OUT4  01
      SUBROUTINEOUT4                                                    OUT4  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,9)                                OUT4  05
  107 FORMAT(12H+          (I2,1H,I3,3H) (I2,1H,I3,1H)/12H          (I2OUT4 107
     1,1H,I3,3H) (I2,1H,I3,1H))                                         OUT4 108
      RETURN                                                            OUT4  09
      END(0,1,0,0,0)                                                    OUT4  11

CHED5    1471 WRB HEADING 5                                             HED5  01
      SUBROUTINEHED5                                                    HED5  03
      WRITEOUTPUTTAPE3,107                                              HED5  05
  107 FORMAT(35H0DIFFERENCE BETWEEN TWO BOND ANGLES)                    HED5 107
      RETURN                                                            HED5  11
      END(0,1,0,0,0)                                                    HED5  13
CFUN5    1471 WRB DIFFERENCE BETWEEN BOND ANGLES                        FUN5  01

      SUBROUTINEFUN5                                                    FUN5  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      FX=FUNA(IN(8))-FUNA(IN(2))                                        FUN5  05
      RETURN                                                            FUN5  07
      END(0,1,0,0,0)                                                    FUN5  09

CHED6    1471 WRB HEADING 6                                             HED6  01
      SUBROUTINEHED6                                                    HED6  03
      WRITEOUTPUTTAPE3,107                                              HED6  05
  107 FORMAT(27H0SUM OF SEVERAL BOND ANGLES)                            HED6 107
      RETURN                                                            HED6  11
      END(0,1,0,0,0)                                                    HED6  13

CPRE6    1471 WRB PRELIMINARY SUBROUTINE 6                              PRE6  01
      SUBROUTINEPRE6                                                    PRE6  03
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      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      J=IN(2)*6+1                                                        PRE6   05
      DO109I=3,J,2                                                       PRE6   07
  109 CALLSETKX(IN(I))                                                   PRE6   09
      RETURN                                                             PRE6   11
      END(0,1,0,0,0)                                                     PRE6   13

CFUN6    1471 WRB SUM OF BOND ANGLES                                     FUN6   01
      SUBROUTINEFUN6                                                     FUN6   03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      N=IN(2)                                                            FUN6   05
      FX=0.0                                                             FUN6   07
      DO111J=1,N                                                         FUN6   09
  111 FX=FX+FUNA(IN(6*J-3))                                              FUN6   11
      RETURN                                                             FUN6   13
      END(0,1,0,0,0)                                                     FUN6   15

COUT6    1471 WRB OUTPUT DESCRIPTION 6                                   OUT6   01
      SUBROUTINEOUT6                                                     OUT6   03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      J=IN(2)*6+2                                                        OUT6   05
      WRITEOUTPUTTAPE3,109,(IN(I),I=3,J)                                 OUT6   07
  109 FORMAT(12H+          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)/(12OUT6  109
     1H           (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)))           OUT6  110
      RETURN                                                             OUT6   11
      END(0,1,0,0,0)                                                     OUT6   13

CFUNB    1471 WRB SET UP MATRIX AND GET EIGENVALUE                       FUNB   01
      SUBROUTINEFUNB(W,Z,Z1)                                             FUNB   03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM    03
      DIMENSIONB(3,3),W(3,3),Y(3)                                        FUNB   05
```

```
      CALLSTOAA                                                         FUNB  07
      CALLBETA(IN(2),B)                                                 FUNB  09
      IF(NG)123,113,123                                                 FUNB  11
  113 CALLMM(B,AA,W)                                                    FUNB  13
      CALLEIGVAL(W,Y)                                                   FUNB  15
      I=IN(4)                                                           FUNB  17
      Z=Y(I)                                                            FUNB  19
      Z1=SQRTF(Z*0.0506605918)                                          FUNB  21
  123 RETURN                                                            FUNB  23
      END(0,1,0,0,0)                                                    FUNB  25

CFUNC    1471 WRB COS ANGLE OF PRINCIPAL AXIS AND VECTOR                FUNC  01
      SUBROUTINEFUNC(C,Z)                                               FUNC  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONW(3,3),X1(3),X2(3),V1(3),V2(3)                           FUNC  05
      CALLFUNB(W,Y,Z)                                                   FUNC  07
      IF(NG)125,111,125                                                 FUNC  09
  111 CALLEIGVEC(W,Y,V1)                                                FUNC  11
      IF(NG)125,115,125                                                 FUNC  13
  115 CALLATOM(IN(5),X1)                                                FUNC  15
      CALLATOM(IN(7),X2)                                                FUNC  17
      IF(NG)125,121,125                                                 FUNC  19
  121 CALLDIFV(X2,X1,V2)                                                FUNC  21
      C=COSVV(V1,V2)                                                    FUNC  23
  125 RETURN                                                            FUNC  25
      END(0,1,0,0,0)                                                    FUNC  27

CFUNX    1471 WRB COS ANGLE OF PRINCIPAL AND CARTESIAN AXES             FUNX 101
      SUBROUTINEFUNX(C,Z)                                               FUNX 103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONW(3,3),V(3),X(3,4),V1(3),V2(3),AX(3,3)                   FUNX 105
      CALLFUNB(W,Y,Z)                                                   FUNX 107
      CALLSTOBB                                                         FUNX 109
      IF(NG)207,113,207                                                 FUNX 111
  113 CALLEIGVEC(W,Y,V)                                                 FUNX 113
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      IF(NG)207,117,207                                                 FUNX 115
  117 DO119I=1,4                                                        FUNX 117
  119 CALLATOM(IN(2*I+4),X(1,I))                                        FUNX 119
      IF(NG)207,123,207                                                 FUNX 121
  123 CALLDIFV(X(1,2),X(1,1),V1)                                        FUNX 123
      CALLDIFV(X(1,4),X(1,3),V2)                                        FUNX 125
      CALLAXES(V1,V2,AX)                                                FUNX 201
      I=IN(5)                                                           FUNX 203
      C=COSVV(V,AX(1,I))                                                FUNX 205
  207 RETURN                                                            FUNX 207
      END(0,1,0,0,0)                                                    FUNX 209

CHED7    1471 WRB HEADING 7                                             HED7  01
      SUBROUTINEHED7                                                    HED7  03
      WRITEOUTPUTTAPE3,107                                              HED7  05
  107 FORMAT(72HORMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL AHED7 107
     1XIS R. ANGSTROMS/25H0              ATOM        R)                 HED7 108
      RETURN                                                            HED7  11
      END(0,1,0,0,0)                                                    HED7  13

CPRE7    1471 WRB PRELIMINARY SUBROUTINE 7                              PRE7  01
      SUBROUTINEPRE7                                                    PRE7  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      CALLSETKB(IN(2))                                                  PRE7  05
      RETURN                                                            PRE7  07
      END(0,1,0,0,0)                                                    PRE7  09

CFUN7    1471 WRB RMS PRINCIPAL DISPLACEMENT                            FUN7  01
      SUBROUTINEFUN7                                                    FUN7  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONW(3,3)                                                   FUN7  05
      CALLFUNB(W,Z,FX)                                                  FUN7  07
      RETURN                                                            FUN7  09
      END(0,1,0,0,0)                                                    FUN7  11
```

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COUT7     1471 WRB OUTPUT DESCRIPTION 7                                    OUT7  01
      SUBROUTINEOUT7                                                       OUT7  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P            COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)       DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)     DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,4)                                   OUT7  05
  107 FORMAT(12H+          (I2,1H,I3,6H)     I1)                           OUT7 107
      RETURN                                                               OUT7  09
      END(0,1,0,0,0)                                                       OUT7  11

CHED8     1471 WRB HEADING 8                                               HED8  01
      SUBROUTINEHED8                                                       HED8  03
      WRITEOUTPUTTAPE3,107                                                 HED8  05
  107 FORMAT(63H0ANGLE BETWEEN PRINCIPAL AXIS R AND VECTOR DEFINED BY TWHED8 107
     1O ATOMS/40H0            ATOM       R          VECTOR)                HED8 108
      RETURN                                                               HED8  11
      END(0,1,0,0,0)                                                       HED8  13

CPRE8     1471 WRB PRELIMINARY SUBROUTINE 8                                PRE8  01
      SUBROUTINEPRE8                                                       PRE8  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P            COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)       DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)     DIM   03
      CALLSETKB(IN(2))                                                     PRE8  05
      DO109I=5,7,2                                                         PRE8  07
  109 CALLSETKX(IN(I))                                                     PRE8  09
      RETURN                                                               PRE8  11
      END(0,1,0,0,0)                                                       PRE8  13

CFUN8     1471 WRB ANGLE BETWEEN PRINCIPAL AXIS AND VECTOR                 FUN8  01
      SUBROUTINEFUN8                                                       FUN8  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P            COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)       DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)     DIM   03
      CALLFUNC(C,Z)                                                        FUN8  05
      FX=ARCCOS(C)                                                         FUN8  07
      RETURN                                                               FUN8  09
      END(0,1,0,0,0)                                                       FUN8  11
```

```
COUT8     1471 WRB OUTPUT DESCRIPTION 8                                    OUT8  01
      SUBROUTINEOUT8                                                       OUT8  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P            COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)       DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)     DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,8)                                   OUT8  05
  107 FORMAT(12H+          (I2,1H,I3,6H)     I1,5H    (I2,1H,I3,3H) (I2,OUT8 107
     11H,I3,1H))                                                           OUT8 108
      RETURN                                                               OUT8  09
      END(0,1,0,0,0)                                                       OUT8  11

CHED9     1471 WRB HEADING 9                                               HED9  01
      SUBROUTINEHED9                                                       HED9  03
      WRITEOUTPUTTAPE3,107                                                 HED9  05
  107 FORMAT(113HORMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL HED9 107
     1AXIS R PROJECTED ON VECTOR DEFINED BY TWO ATOMS. ANGSTROMS/40H0      HED9 108
     2          ATOM       R          VECTOR)                              HED9 109
      RETURN                                                               HED9  11
      END(0,1,0,0,0)                                                       HED9  13

CFUN9     1471 WRB PRINCIPAL AXIS PROJECTED ON VECTOR                      FUN9  01
      SUBROUTINEFUN9                                                       FUN9  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P            COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)       DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)     DIM   03
      CALLFUNC(C,Z)                                                        FUN9  05
      FX=C*Z                                                               FUN9  07
      RETURN                                                               FUN9  09
      END(0,1,0,0,0)                                                       FUN9  11

CHED10    1471 WRB HEADING 10                                              HED10 01
      SUBROUTINEHED10                                                      HED10 03
      WRITEOUTPUTTAPE3,107                                                 HED10 05
  107 FORMAT(85H0ANGLE BETWEEN PRINCIPAL AXIS R AND AXIS I OF CARTESIAN HED10107
     1SYSTEM DEFINED BY TWO VECTORS/45H0            ATOM     R   I   DEFIHED10108
     2NING VECTORS)                                                        HED10109
      RETURN                                                               HED10 11
      END(0,1,0,0,0)                                                       HED10 13
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CPRE10    1471 WRB PRELIMINARY SUBROUTINE 10                                PRE10 01
      SUBROUTINEPRE10                                                       PRE10 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P             COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)        DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)      DIM   03
      CALLSETKB(IN(2))                                                      PRE10 05
      DO109I=6,12,2                                                         PRE10 07
  109 CALLSETKX(IN(I))                                                      PRE10 09
      RETURN                                                                PRE10 11
      END(0,1,0,0,0)                                                        PRE10 13

CFUN10    1471 WRB ANGLE BETWEEN PRINCIPAL AND CARTESIAN AXES               FUN10 01
      SUBROUTINEFUN10                                                       FUN10 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P             COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)        DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)      DIM   03
      CALLFUNX(C,Z)                                                         FUN10 05
      FX=ARCCOS(C)                                                          FUN10 07
      RETURN                                                                FUN10 09
      END(0,1,0,0,0)                                                        FUN10 11

COUT10    1471 WRB OUTPUT DESCRIPTION 10                                    OUT10 01
      SUBROUTINEOUT10                                                       OUT10 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P             COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)        DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)      DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,13)                                   OUT10 05
  107 FORMAT(12H+          (I2,1H,I3,4H)   I1,I3,4H   (I2,1H,I3,3H) (I2,OUT10106
     11H,I3,1H)/30H                                (I2,1H,I3,3H) (I2,1H,I3,OUT10107
     21H))                                                                  OUT10108
      RETURN                                                                OUT10 09
      END(0,1,0,0,0)                                                        OUT10 11

CHED11    1471 WRB HEADING 11                                               HED11 01
      SUBROUTINEHED11                                                       HED11 03
      WRITEOUTPUTTAPE3,107                                                  HED11 05
  107 FORMAT(101HORMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL HED11107
     1AXIS R PROJECTED ON AXIS I OF CARTESIAN SYSTEM/34H DEFINED BY TWO HED11108
     2VECTORS. ANGSTROMS/45H0            ATOM     R  I   DEFINING VECTORHED11109
```

```
     3S)                                                                HED11110
      RETURN                                                            HED11 11
      END(0,1,0,0,0)                                                    HED11 13

CFUN11   1471 WRB PRINCIPAL AXIS PROJECTED ON CARTESIAN AXIS            FUN11 01
      SUBROUTINEFUN11                                                   FUN11 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      CALLFUNX(C,Z)                                                     FUN11 05
      FX=C*Z                                                            FUN11 07
      RETURN                                                            FUN11 09
      END(0,1,0,0,0)                                                    FUN11 11

CFUNR    1471 WRB MEAN SQUARE RADIAL DISPLACEMENT                       FUNR 101
      SUBROUTINEFUNR(I,RSQ)                                             FUNR 103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONB(3,3),BAA(3,3)                                          FUNR 105
      CALLSTOAA                                                         FUNR 107
      CALLBETA(I,B)                                                     FUNR 109
      CALLMM(B,AA,BAA)                                                  FUNR 111
      RSQ=TRACE(BAA)*0.0506605918                                       FUNR 113
      RETURN                                                            FUNR 115
      END(0,1,0,0,0)                                                    FUNR 117

CFUNCR   1471 WRB COMPUTE QUANTITIES FOR MEAN BOND DISTANCE             FUNCR 01
      SUBROUTINEFUNCR(C,R)                                              FUNCR 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONC(2),X(3,2),V(3)                                         FUNCR 05
      DO115I=1,2                                                        FUNCR 07
      CALLFUNR(IN(2*I),RSQ)                                             FUNCR 09
      CALLFUNXI(IN(2*I),IN(2),XISQ)                                     FUNCR 11
      C(I)=RSQ-XISQ                                                     FUNCR 13
  115 CALLATOM(IN(2*I),X(1,I))                                          FUNCR 15
      CALLDIFV(X(1,2),X(1,1),V)                                         FUNCR 17
```

```
      R=SQRTF(VMV(V,AA,V))                                              FUNCR 19
      RETURN                                                            FUNCR 21
      END(0,1,0,0,0)                                                    FUNCR 23

CFUNXI    1471 WRB MS DISPLACEMENT IN GIVEN DIRECTION                   FUNXI101
      SUBROUTINEFUNXI(I,J,XISQ)                                         FUNXI103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONI(2),J(4),B(3,3),X1(3),X2(3),V(3),BAA(3,3),AABAA(3,3)    FUNXI105
      CALLSTOAA                                                         FUNXI107
      CALLBETA(I,B)                                                     FUNXI109
      CALLATOM(J,X1)                                                    FUNXI111
      CALLATOM(J(3),X2)                                                 FUNXI113
      IF(NG)207,117,207                                                 FUNXI115
  117 CALLDIFV(X2,X1,V)                                                 FUNXI117
      D=VMV(V,AA,V)                                                     FUNXI119
      IF(D)123,123,201                                                  FUNXI121
  123 NG=10                                                             FUNXI123
      GOTO207                                                           FUNXI125
  201 CALLMM(B,AA,BAA)                                                  FUNXI201
      CALLMM(AA,BAA,AABAA)                                              FUNXI203
      XISQ=VMV(V,AABAA,V)*0.0506605918/D                                FUNXI205
  207 RETURN                                                            FUNXI207
      END(0,1,0,0,0)                                                    FUNXI209

CHED12    1471 WRB HEADING 12                                           HED12 01
      SUBROUTINEHED12                                                   HED12 03
      WRITEOUTPUTTAPE3,107                                              HED12 05
  107 FORMAT(83HORMS COMPONENT OF THERMAL DISPLACEMENT IN DIRECTION DEFIHED12107
     1NED BY TWO ATOMS. ANGSTROMS/40H0            ATOM                 VHED12108
     2ECTOR)                                                            HED12109
      RETURN                                                            HED12 11
      END(0,1,0,0,0)                                                    HED12 13

CPRE12    1471 WRB PRELIMINARY SUBROUTINE 12                            PRE12 01
      SUBROUTINEPRE12                                                   PRE12 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
```

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```
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      CALLSETKB(IN(2))                                                  PRE12 05
      DO109I=4,6,2                                                      PRE12 07
  109 CALLSETKX(IN(I))                                                  PRE12 09
      RETURN                                                            PRE12 11
      END(0,1,0,0,0)                                                    PRE12 13

CFUN12   1471 WRB RMS DISPLACEMENT LN GIVEN DIRECTION                   FUN12 01
      SUBROUTINEFUN12                                                   FUN12 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      CALLFUNXI(IN(2),IN(4),XISQ)                                       FUN12 05
      FX=SQRTF(XISQ)                                                    FUN12 07
      RETURN                                                            FUN12 09
      END(0,1,0,0,0)                                                    FUN12 11
COUT12   1471 WRB OUTPUT DESCRIPTION 12                                 OUT12 01
      SUBROUTINEOUT12                                                   OUT12 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,7)                                OUT12 05
  107 FORMAT(12H+          (I2,1H,I3,12H)          (I2,1H,I3,3H) (I2,1H,OUT12107
     1I3,1H))                                                           OUT12108
      RETURN                                                            OUT12 09
      END(0,1,0,0,0)                                                    OUT12 11

CHED13   1471 WRB HEADING 13                                            HED13 01
      SUBROUTINEHED13                                                   HED13 03
      WRITEOUTPUTTAPE3,107                                              HED13 05
  107 FORMAT(51HORMS RADIAL THERMAL DISPLACEMENT OF ATOM. ANGSTROMS)    HED13107
      RETURN                                                            HED13 11
      END(0,1,0,0,0)                                                    HED13 13


CFUN13   1471 WRB RMS RADIAL DISPLACEMENT                               FUN13 01
      SUBROUTINEFUN13                                                   FUN13 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
```

```
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM    03
      CALLFUNR(IN(2),RSQ)                                               FUN13  05
      FX=SQRTF(RSQ)                                                     FUN13  07
      RETURN                                                            FUN13  09
      END(0,1,0,0,0)                                                    FUN13  11

COUT13   1471 WRB OUTPUT DESCRIPTION 13                                 OUT13  01
      SUBROUTINEOUT13                                                   OUT13  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM    03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,3)                                OUT13  05
  107 FORMAT(12H+          (I2,1H,I3,1H))                               OUT13107
      RETURN                                                            OUT13  09
      END(0,1,0,0,0)                                                    OUT13  11

CHED14   1471 WRB HEADING 14                                            HED14  01
      SUBROUTINEHED14                                                   HED14  03
      WRITEOUTPUTTAPE3,107                                              HED14  05
  107 FORMAT(88H0INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. SECOHED14107
     1ND ATOM ASSUMED TO RIDE ON FIRST)                                 HED14108
      RETURN                                                            HED14  11
      END(0,1,0,0,0)                                                    HED14  13

CPRE14   1471 WRB PRELIMINARY SUBROUTINE 14                             PRE14  01
      SUBROUTINEPRE14                                                   PRE14  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM    01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM    01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM    03
      DO109I=2,4,2                                                      PRE14  05
      CALLSETKX(IN(I))                                                  PRE14  07
  109 CALLSETKB(IN(I))                                                  PRE14  09
      RETURN                                                            PRE14  11
      END(0,1,0,0,0)                                                    PRE14  13

CFUN14   1471 WRB MEAN BOND DISTANCE ASSUMING RIDING                    FUN14  01
```

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```
      SUBROUTINEFUN14                                                   FUN14 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONC(2)                                                     FUN14 05
      CALLFUNCR(C,R)                                                    FUN14 07
      FX=R+(C(2)-C(1))/(2.0*R)                                          FUN14 09
      RETURN                                                            FUN14 11
      END(0,1,0,0,0)                                                    FUN14 13

CHED15   1471 WRB HEADING 15                                            HED15 01
      SUBROUTINEHED15                                                   HED15 03
      WRITEOUTPUTTAPE3,107                                              HED15 05
  107 FORMAT(87H0INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. ATOMHED15107
     1S ASSUMED TO MOVE INDEPENDENTLY)                                  HED15108
      RETURN                                                            HED15 11
      END(0,1,0,0,0)                                                    HED15 13

CFUN15   1471 WRB MEAN INTERATOMIC DISTANCE ASSUMING INDEPENDENT MOTION FUN15 01
      SUBROUTINEFUN15                                                   FUN15 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONC(2)                                                     FUN15 05
      CALLFUNCR(C,R)                                                    FUN15 07
      FX=R+(C(2)+C(1))/(2.0*R)                                          FUN15 09
      RETURN                                                            FUN15 11
      END(0,1,0,0,0)                                                    FUN15 13
```

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by D. J. Wehe, W. R. Busing and H. A. Levy

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OR ABS

A FORTRAN PROGRAM FOR CALCULATING SINGLE CRYSTAL ABSORPTION CORRECTIONS

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ORNL-TM- 229

OR ABS

A FORTRAN PROGRAM FOR CALCULATING SINGLE CRYSTAL ABSORPTION CORRECTIONS

by

D. J. Wehe, W. R. Busing, and H. A. Levy

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ABSTRACT

This memorandum describes a Fortran program for calculating the absorption correction to be applied to single crystal x-ray or neutron diffraction intensity measurements. Instructions are included for using the program which is available from the authors in the form of symbolic punched cards.

INTRODUCTION

The derivation of structure factors from integrated intensity measurements in X-ray or neutron diffraction usually requires a correction for absorption of radiation in the specimen. Tabulated values of this correction, expressed as the ratio of integrated intensity yielded by an absorbing specimen to that yielded by an hypothetical non-absorbing specimen of equal volume, are available for cylindrical (Bradley, 1935) and spherical (Evans and Ekstein, 1952) sample shapes. For accurate measurement of structure factors, the specimen is often reduced to one of these simple forms.

However, for a number of reasons, it frequently proves to be undesirable or difficult to shape a sample. The size and shape of available crystals may not permit cutting a sphere or cylinder large enough to give satisfactory intensities. Physical properties such as anisotropic resistance to grinding, or ease of cleavage or fracture may make shaping difficult. Furthermore, a cylindrical specimen may be used in only one orientation; while a spherical specimen obviates this difficulty, it may not permit optimum use of a beam with a long narrow cross section such as is usual in neutron diffraction spectrometers.

Several methods of correcting for absorption in samples of other shapes have been reported by Hendershot (1937), Albrecht (1939), Howells (1950) and Evans (1952), but all of them appear to be rather laborious. The availability of high-speed computers now makes possible the rapid calculation of the absorption correction factor for each reflection from a crystal of essentially arbitrary shape. The program to be described is similar to one prepared for the Oak Ridge computer, the Oracle (Busing and Levy, 1956).

MATHEMATICAL METHOD

It is assumed that the crystal is bounded by n plane surfaces and thus is described by a set of inequalities

$$a_s x + b_s y + c_s z - d_s \geq 0, \qquad s = 1, 2, \ldots, n, \tag{1}$$

with coefficients a_s, b_s, c_s, d_s chosen so that the inequalities are all satisfied only if the point x, y, z lies inside or on the surface of the crystal. This is a satisfactory description if there are no re-entrant angles between bounding planes, a condition which is assumed for this treatment. Cartesian coordinate axes for this description are those used to describe the angles which give the directions of the primary and diffracted beam. Two configurations are discussed under the subroutine ANGLE.

The factor to be computed is given by

$$A = \int (1/V)\exp[-\mu(r_\alpha + r_\beta)]dV, \tag{2}$$

where the integration is over the volume of the crystal, V, and where μ is the linear absorption coefficient, r_α the path length along the primary beam direction, and r_β that along the diffracted beam direction. In this program the integral is evaluated numerically using the method of Gauss (see, for example, Margenau and Murphy, 1943, p. 462) which will be described first for a one-dimensional integration. The method approximates the integral by a weighted sum of m terms:

$$\int_a^b g(x)dx \approx (b-a) \sum_{i=1}^{m} R_i g(x_i) ,$$

where

$$x_i = a+(b-a)u_i$$

and where the u_i's and R_i's are fractional constants which depend only on m, and their values are available for $m \leq 16$ (Lowan, Davids, and Levenson, 1942). The u_i's determine the points, x_i, at which the integrand

is evaluated, while the R_i's are the relative weights of the terms in the sum.

For triple integration, the approximation becomes

$$\int_a^b dx \int_{c(x)}^{d(x)} dy \int_{e(x,y)}^{f(x,y)} g(x,y,z)dz \approx$$

$$\sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{k=1}^{m} (b-a)[d(x_i)-c(x_i)][f(x_i,y_j)-e(x_i,y_j)]R_iR_jR_k g(x_i,y_j,z_k),$$

where

$$x_i = a+(b-a)u_i, \tag{3}$$

$$y_j = c(x_i)+[d(x_i)-c(x_i)]u_j, \tag{4}$$

$$z_k = e(x_i,y_j)+[f(x_i,y_j)-e(x_i,y_j)]u_k \ . \tag{5}$$

Tests of the method for conditions typical of neutron diffraction studies indicate that an m of 8 is satisfactory. The problem of determining A then reduces to finding the limits of integration, a, b, $c(x_i)$, $d(x_i)$, $e(x_i,y_j)$, and $f(x_i,y_i)$ and evaluating $g(x_i,y_j,z_k) = (1/V)\exp[-\mu(r_\alpha+r_\beta)]$.

In order to find a and b, the lower and upper limits on x, the routine first takes all possible combinations of three of the n planes which bound the crystal and solves for the coordinates of their intersections. Because there are no re-entrant angles between the faces, those intersections which are not corners of the crystal must lie outside of it. These are distinguished from the corners by rejecting points which fail to satisfy any one of the inequalities (1). The smallest and largest x values in the remaining set are then taken as a and b, respectively.

For a given value of x_i, the limits on y are found in a similar way by solving the equations of all possible pairs of faces, subject to the condition that $x = x_i$. Points outside the crystal are again rejected

and the smallest and largest y values remaining are taken as $c(x_i)$ and $d(x_i)$, respectively. The limits on z are determined in an analogous way for given values of x_i and y_j.

For a point x_i, y_j, z_k, the function $\exp[-\mu(r_\alpha+r_\beta)]$ is evaluated as follows. The distance from this point to the intersection of the primary beam with a face s of the crystal (or its extension) specified by one of the inequalities (1) is given by

$$r_{\alpha s} = \frac{d_s - a_s x_i - b_s y_j - c_s z_k}{a_s \gamma_{\alpha x} + b_s \gamma_{\alpha y} + c_s \gamma_{\alpha z}} \tag{6}$$

where the γ_α's are the direction cosines of a vector parallel to the primary beam and directed toward its source. This quantity is positive if the intersection lies toward the source of the primary beam from (x_i, y_j, z_k) and negative if it lies away from the source. The desired path length, r_α, is the smallest positive quantity of the set $r_{\alpha s}$. Similarly, the path length r_β is the smallest positive quantity in the set

$$r_{\beta s} = \frac{d_s - a_s x_i - b_s y_j - c_s z_k}{a_s \gamma_{\beta x} + b_s \gamma_{\beta y} + c_s \gamma_{\beta z}} \tag{7}$$

where the γ_β's are the direction cosines of the diffracted beam. The exponential is then evaluated in a straightforward way.

OUTLINE OF PROGRAM

It is usually necessary to determine the values of A for many reflections from a given crystal, and, sometimes, for several values of μ. The program avoids much repetition by calculating only once the limits of integration a, b, c, d, e, and f and the points of integration x_i, y_i, z_i. These determine the nm^3 numerators of Equations (6) and (7) and the m^3 weights of integration

$$R_{ijk} = (b-a)(d-c)(f-e)R_i R_j R_k \ ,$$

which are saved in a block of core, or on magnetic tape, if necessary. In the second part of the program the numerators are used to determine A for each reflection.

The amount of core available for data storage is determined by a subroutine (which must be the last one loaded) which determines the length of the code, size of machine, and amount of upper core unavailable. The size of the numerator block is then computed as the largest factor of m^2 possible, considering the number of faces, number of points of integration, and number of μ. In some cases, all numbers can be stored in fast storage, and no magnetic tape is used.

The majority of the input is read by two subroutines, one of which describes the shape of the crystal (FACE) and the other of which describes the angles of the reflection (ANGLE). Thus the user may describe his crystal and reflections in any convenient manner and supply a subroutine which will convert his input into the desired data.

The calculations begin with the determination of the limits a and b as described earlier, and the values of x_i are then found from (3), using the tabulated u's. For each x_i the limits c and d are then calculated and the values of y_j found from (4). Finally, for each combination x_i, y_j the limits e and f are determined and the values z_k taken from (5). Given the coordinates x_i, y_j, and z_k the n numerators of (6) and (7) may be calculated and stored, together with the weight which is determined using the tabulated values of R. The crystal volume, which is simply the sum of all the weights, is also determined in this part of the code.

In the second part of the program remaining storage is used for reflection data for several reflections. By performing the calculation

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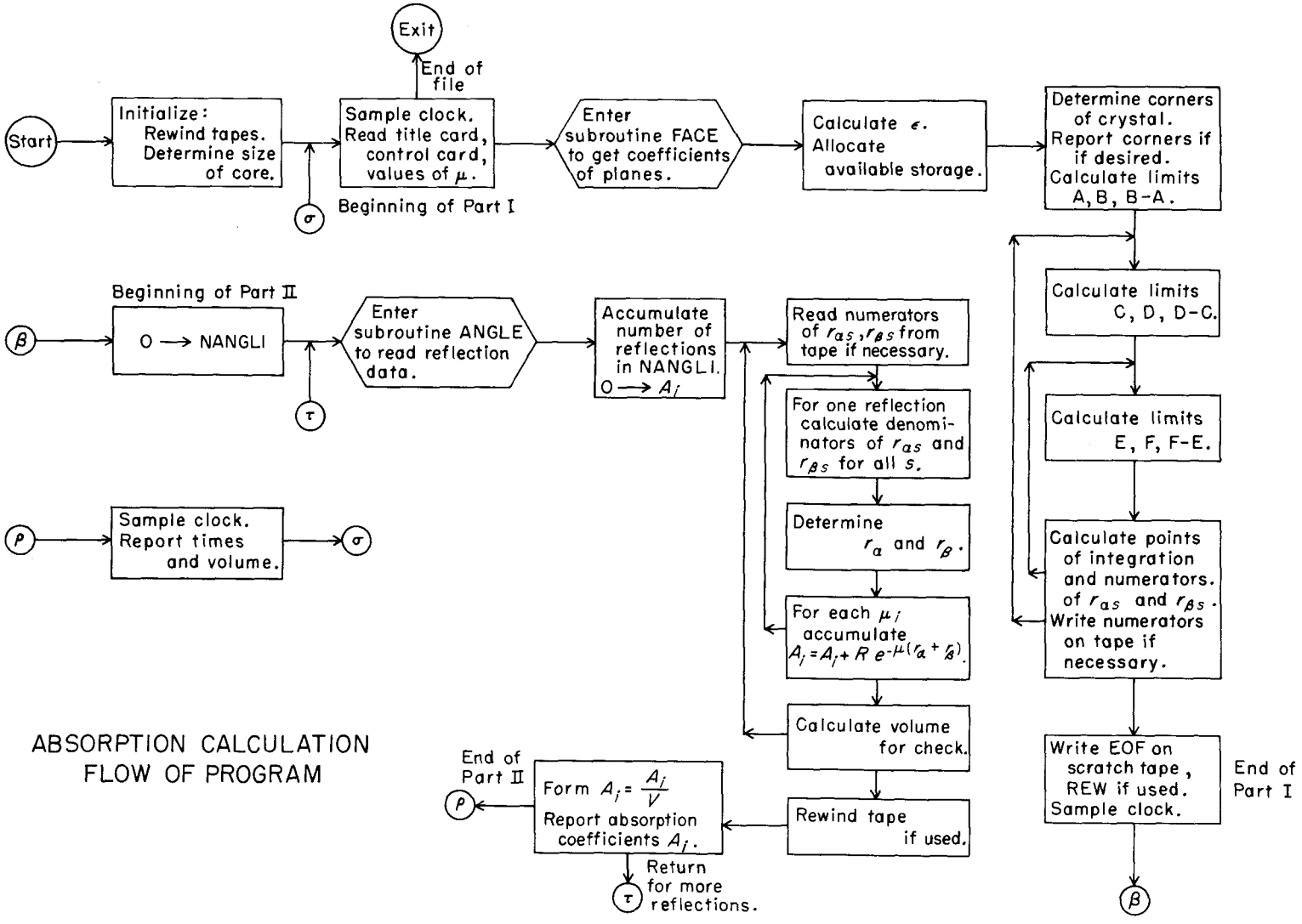

ABSORPTION CALCULATION
FLOW OF PROGRAM

for several reflections at a time, magnetic tape handling is minimized. As each block of numerators is read from magnetic tape, the 2n denominators of (6) and (7) are calculated. The distances r_α and r_β are determined, and appropriate contribution added to the sums for each reflection in core.

An on-line clock helps the user to estimate the time required for each run. The clock is sampled at the beginning of the program, at the end of the first part, and at the end of the problem. The last page of output for any crystal is a log giving the crystal identification, date, n, m, number of blocks of magnetic tape used, the number of values of μ, the number of reflections, and the time required for the two parts of the program. The volume of the crystal is also reported at this time for checking purposes.

Several checks are made during the calculations. Should the program fail a check, a notation is made on the output as to the nature of the error and the extent of the calculation before the run is terminated.

PREPARATION OF THE PROGRAM DECK

There are many features of this program which depend either on the arrangement of the diffraction equipment used or on the requirements of the computing installation. For this reason it is expected that in most cases minor modifications will have to be made before the program can be used. The program is therefore being transmitted in the form of symbolic cards, although column-binary cards are also available on request.

The following is a list of the subprograms which should be included in the assembled program deck. Several of them are discussed in more

detail in the next section.

Subprogram	Identification of Symbolic Cards	Remarks
1. Fortran II BSS loader		
2. Main program	P1 000-336	
3. Fortran II library subroutines		Not punched automatically on compiling
4. GAUSØL	G 337-384	
5. IDØUT	ID 385-391	
6. ØCØR	ØC 392-407	
7. EPSR	E1 408-413	
8. CLØCK	C1 414-421 C2 422-488	Alternative versions
9. ANGLE	A1 489-533 A2 534-591	Alternative versions
10. FACE	F1 592-630	
11. SIZE	S 631-659	Must be last subprogram
12. Fortran II transfer card		
13. Gaussian constants		
(a) Number of points	M 660	
(b) Gaussian weights	R1-2 661-662	These constants are read by the program as data cards.
(c) Gaussian points	U1-2 663-664	

DETAILS OF THE SUBPROGRAMS

Subroutines ERRØR and EXIT

The Oak Ridge installation requires that a run be terminated in one of three ways. The Fortran input routine has been modified to recognize an end of file on the input tape as the normal end of the run. An entrance

into EXIT subroutine terminates the problem in a similar fashion. An entrance into ERRØR implies that an octal dump of core is desired. The user must supply EXIT and ERRØR routines which conform to local standards.

Subroutine SIZE

This subroutine determines the number of cells available in core for storage of data.

The routine labelled S in columns 77-78 should be usable on a IBM 704, 709, or 7090 of any size. In the decrement of SIZE + 5 is the amount of upper core not available to the program (205 for Oak Ridge). The routine uses the fact that it is the last subprogram loaded to determine the length of the code and the part of lower core not available to the program.

If a new routine is written it must use the calling sequence

CALL SIZE (NS)

and place the number of cells available for data storage in the decrement of NS as an integer. The main program will subtract from this the number of cells used by variables and fixed arrays in CØMMØN, thus determining the length of the array DATA.

Subroutine CLØCK

The routine CLØCK is entered three times for each crystal to provide the user with the date of the run and the time required for Parts I and II of the program.

Two subroutines are provided. CLØCK with the identification C1 in columns 77-78 is a dummy which places blanks in DATE and gives zero for the time in T. It may be used when no on line clock is available.

The second routine, identified by C2 in columns 77-78, reads a Chrono-log digital clock model 2704-1, which has been connected to the 716 on-line printer control panel according to drawing 2704-9 which is furnished with the clock by the Chrono-log Corporation of Philadelphia 31, Pennsylvania. In addition to the wiring shown on the drawing, a wire is run from the load switching circuit (clock cable wire 50) through a filter into the sense entry hub. The read out of the clock is under control of printer sense exit six. The date of the run is given in BCD in DATE in the form mmddyy, mm being the month, dd, the day, and yy, the year. The time of the run in 10's of seconds is placed in the decrement of IT.

The calling sequence is CALL CLØCK (IT, DATE). The routine, in general, must place 6 BCD characters in DATE and an integer in the decrement of IT. The main program will report elapsed time as $IT-IT_1$ (IT_1 obtained on an earlier entry).

Subroutine EPSR

When determining the corners of the crystal, it is necessary, because of rounding errors, to accept a point as on the crystal surface if

$$a_s x + b_s y + c_s z - d_s + \epsilon \geq 0$$

for some small $\epsilon > 0$. If the program is not giving correct results, it is possible that an examination of the corners of the crystal that were found would indicate that an adjustment of the tolerance ϵ is required.

The main program reads an input parameter EPS. The subroutine EPSR must calculate EPS1 which is to be used as ϵ in the above inequality. The subprogram identified by E1 in columns 77-78 simply sets EPS1 equal to EPS.

Subroutine FACE

This subroutine provides the program with the 4n coefficients a_s, b_s, c_s, and d_s defined in Equation (1). The subroutine includes

the reading of input, the calculation of coefficients, and the reporting of input or coefficients, if desired.

The subroutine identified by F1 in columns 77-78 reads the following input cards via tape 10:

Card 1: Columns 1-5: N, the number of faces of the crystal, $N < 100$

6-10: NØP. A number other than zero implies that the input is to be reported.

Cards 2, ..., N + 1:	Columns 1-10	a_s	
	11-20	b_s	As defined in Equation (1)
	21-30	c_s	
	31-40	d_s	

The coefficients a_s, b_s, c_s, d_s must be given with references to a coordinate system which is consistent with the angle description (see below). If NØP is not zero, the title card read in the main program and a list of the coefficients a, b, c, and d are reported on tape 9.

To write a different subroutine FACE, the following conventions should be observed:

(1) The subroutine is entered with the statement CALL FACE (IDENT, N, DATA, NCØF, DATE).

(2) The subroutine should include the reading and reporting of all data needed to define the crystal faces. Output on tape K may be headed with the title and date of run by using the statement CALL IDØUT (IDENT, DATE, K).

(3) The number of faces is stored by the subroutine as an integer in the decrement of N.

(4) The 4n coefficients are stored in DATA (NCØF) through DATA (NCØF + 4N - 1) in the order a_1, b_1, c_1, d_1, a_2, etc. At least

2N cells beyond DATA (NCØF + 4N - 1) are available to the subroutine for temporary storage.

(5) If sense lights 1 and 2 are used, they must be turned off before returning to the main program.

Subroutine ANGLE

This subroutine gives the main program an identification for each reflection and calculates the direction cosines $\gamma_{\alpha x}$, $\gamma_{\alpha y}$, $\gamma_{\alpha z}$, $\gamma_{\beta x}$, $\gamma_{\beta y}$, and $\gamma_{\beta z}$ used in Equations (6) and (7). Two versions of this subroutine have been provided.

The subprogram identified by A1 in columns 77-78 deals with reflections in one zone. Let the z-axis be parallel to the zone axis being studied, and let the x-axis lie in a crystal plane which will be used as a reference plane for all the reflections being studied. The y-axis is chosen to give a right handed coordinate system. The configuration of the crystal and the spectrometer for a given reflection is specified by Θ, the Bragg angle, and χ, the interplanar angle with respect to the reference plane. (See Busing and Levy, 1957, Fig. 1.) From these the routine calculates

$$\alpha = \chi + \Theta + \pi$$

and

$$\beta = \chi - \Theta$$

which define the reverse directions of the primary beam and the forward direction of the diffracted beam. The direction cosines required by the main program are

$$\gamma_{\alpha x} = \cos \alpha \qquad \gamma_{\beta x} = \cos \beta$$

$$\gamma_{\alpha y} = \sin \alpha \qquad \gamma_{\beta y} = \sin \beta$$

$$\gamma_{\alpha z} = 0 \qquad \gamma_{\beta z} = 0.$$

Input for each reflection consists of a BCD identification and the angles Θ and X. This input will be reported as BCD output on tape 6 if desired.

The subprogram identified A2 in columns 77-78 is for use with the Oak Ridge automatic neutron diffractometer or with the General Electric single crystal orienter. The geometry for each reflection is defined by three angles: Θ, the Bragg angle, and X and ϕ, the orienter settings.

The crystal may be mounted on the orienter in an arbitrary way (but the values of X and ϕ depend on the way in which it is mounted). The coordinate system to which the crystal faces are referred is chosen as shown in Fig. 1. Assume the instrument to be in position for a hypothetical reflection for which $X = \phi = 0$ and Θ has a small positive value. The x-axis is then chosen as the normal to this hypothetical reflecting plane, and the z-axis is taken parallel to the ϕ-axis in the direction away from the goniometer mount. The y-axis is then parallel to the X-axis in a direction chosen so that the coordinate system will be right-handed. For the Oak Ridge diffractometer (Fig. 1a) the y-axis will point in the general direction of the primary and diffracted beams, while for the General Electric orienter (Fig. 1b) the opposite will be true. (Note that for the General Electric orienter the roles of the primary and diffracted beams are interchanged but this has no effect on the calculation.)

The subprogram evaluates the required direction cosines as follows:

$$\gamma_{\alpha x} = \cos X \cos \phi \sin \Theta + \sin \phi \cos \Theta \qquad \gamma_{\beta x} = \cos X \cos \phi \sin \Theta - \sin \phi \cos \Theta$$

$$\gamma_{\alpha y} = \cos X \sin \phi \sin \Theta - \cos \phi \cos \Theta \qquad \gamma_{\beta y} = \cos X \sin \phi \sin \Theta + \cos \phi \cos \Theta$$

$$\gamma_{\alpha z} = \sin X \sin \Theta \qquad \gamma_{\beta z} = \sin X \sin \Theta.$$

Input for the subroutine consists of a BCD identification and the angles Θ, X, and ϕ. If desired, the identification and input angles will be reported as BCD output on tape 6.

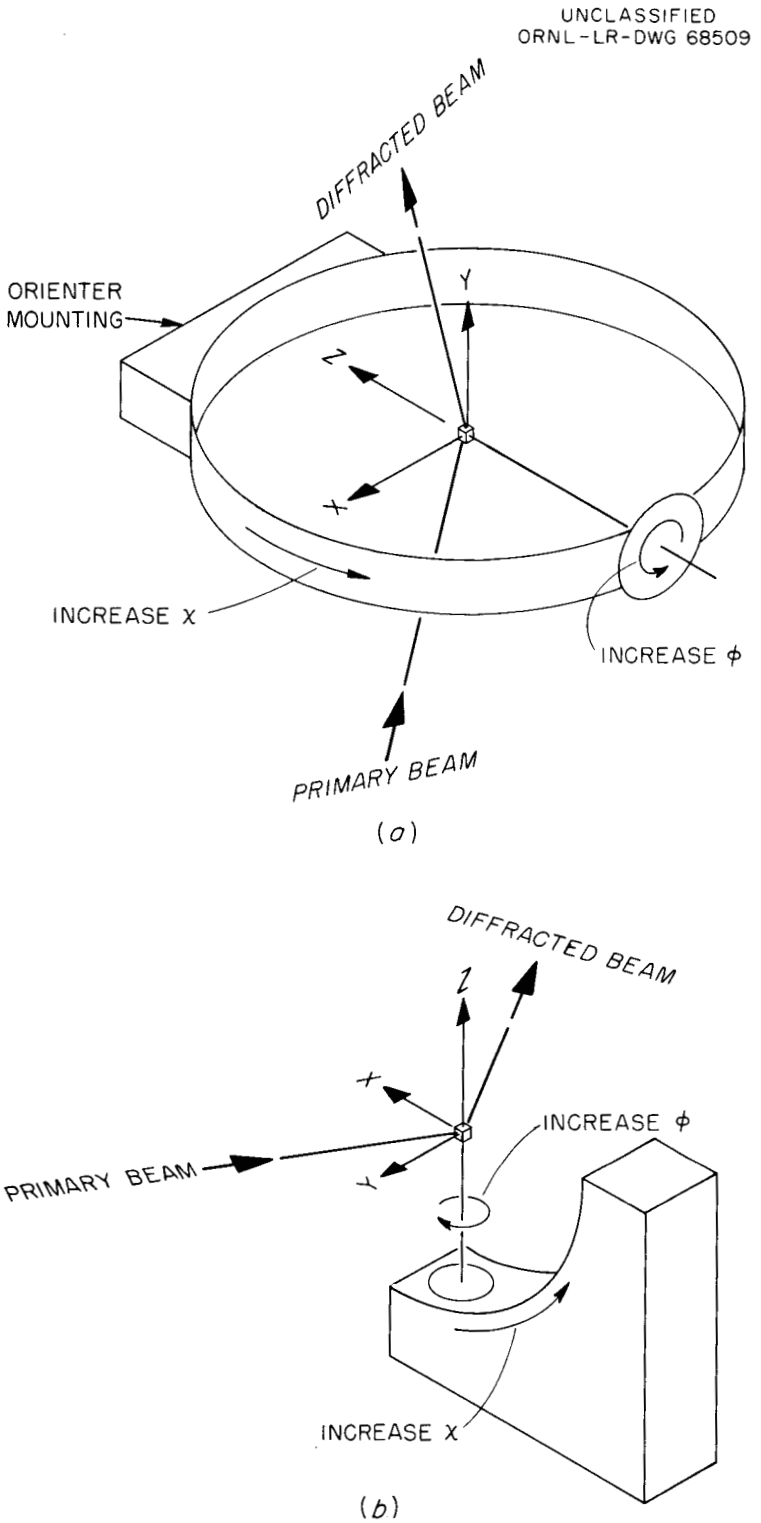

Figure 1. The angles and coordinate systems for (a) the Oak Ridge automatic diffractometer and (b) the General Electric single crystal orienter. The axes to which the crystal faces are referred are shown for $X = \phi = 0$.

To write ANGLE subroutines for other crystal orientations, the following specifications must be adhered to.

(1) Entry is by the statement

CALL ANGLE (IDENT, DATA, IANG, NANGL, DATE, NANGL1).

The arguments are defined below.

(2) The routine must read all of the input needed to define the reflections. If the user wishes to report this input or other results, this must be done within the subroutine. Tape 6 is rewound only once at the beginning of the main program and may be used for output by ANGLE.

(3) The crystal identification is found in the twelve word BCD array IDENT, and the date is in BCD in DATE. These may be reported by the subroutine on tape K, together with a skip to Channel 1, by the statement

CALL IDOUT (IDENT, DATE, K)

(4) The first entry into ANGLE may be distinguished from subsequent entries, since NANGL1 is zero only for the first entry.

(5) The program is more efficient on small machines if the data for several reflections are in core as a group. The maximum number of reflections that can be processed in such a group is found in NANGL on the first entry only. The subroutine should set NANGL to the actual number of reflections for which the angle data has been stored in core.

(6) Data for the reflections must be stored in the one-dimensional array DATA beginning at DATA (IANG). At exit, the data should be stored in groups of seven words in the following order:

1st word: Six BCD characters to identify the following reflection

2nd word: γ_{0x}

3rd word:	$\gamma_{\alpha y}$	direction cosines for primary beam
4th word:	$\gamma_{\alpha z}$	
5th word:	$\gamma_{\beta x}$	direction cosines for diffracted beam
6th word:	$\gamma_{\beta y}$	
7th word:	$\gamma_{\beta z}$	

NANGL words of storage in DATA following the reflection data may be used as temporary storage.

(7) When the data for the last reflection has been read into core, the subroutine must turn on sense light 1.

RESTRICTIONS AND MACHINE REQUIREMENTS

The following restrictions and requirements apply to the program as written. Most of them can be changed by making the appropriate modification. Equipment needed:

(1) The source program may be assembled and run on an IBM 704, 709, or 7090. At least 8,192 words of storage are required.

(2) At most 4 tape units are required. One for scratch (tape 2), one for input (tape 10), and two for output. (Main output is on tape 9, but reflection angles are put out via tape 6, if desired).

(3) A card-to-tape unit is used to prepare the input tape.

(4) All output is printed off-line.

(5) An on-line clock is used for timing.

Program restrictions:

(1) Uses sense lights 1 and 2.

(2) Does not use sense switches.

(3) Output gives 56 lines per page. It should be listed under program control. Automatic overflow switch should be off if the carriage tape has less than 56 lines.

(4) Program does not rewind input or output tapes. No end of file is written on the main output tape by the program at the end of a run.

TIMING

The machine time for a problem may be estimated from the expression

$$T = (C_1 N + C_2)R .$$

Here T is the time in seconds, N is the number of crystal faces, and R is the number of reflections for which the correction is to be calculated. Preliminary tests on an IBM 704 computer show that $C_1 = 1.1$ seconds per face per reflection, and $C_2 = 2.0$ seconds per reflection if intermediate magnetic tape storage is used, or $C_2 = 0$ when magnetic storage is not needed. Usually magnetic storage will be needed with an 8K memory but not with a 32 K memory.

DATA INPUT

1. Title card. FORMAT (12A6)

   cols.
   1-72 Any 72 Hollerith characters. This title will head each section of the output.

2. Card control. FORMAT (I5, E15.8, I5)

   cols.
   1-5 NMU, the number of absorption coefficients. $1 \leq NMU \leq 6$.

   6-20 EPS, the increment used to compensate for round-off error in determining the limits of integration. For crystals of dimensions of the order of 0.1 and face equations with coefficients of the order of 1 an EPS of 10^{-6} (i.e. 1.0E-6) will usually be satisfactory.

   21-25 KØ = 0 if output of coordinates of crystal corners is not desired. KØ = 1 to obtain this output.

3. Absorption coefficients. FORMAT (6E10.8)

cols.	
1-10	MU(K), the absorption coefficients to be used in calculating
11-20 etc.	A for each reflection. The number of MU(K) must be NMU given on the control card above.

4. Input for FACE routine F1.

a. Face control card. FØRMAT (2I5)

col.	
1-5	N, the number of faces of the crystal. $4 \leq N < 100$
6-10	NØP = 0 if output of the coefficients a, b, c, d are not desired; NØP = 1 if this output is desired.

b. Coefficients of planes describing faces of crystal. FØRMAT (4E10.8)

The number of cards is equal to N, the number of faces of the crystal.

col.	
1-10	a.
11-20	b.
21-30	c.
31-40	d.

Note that the coordinate system to which these equations refer must be consistent with the angle description used below.

5. Input for ANGLE routine A1. (Used for zero level reflections).

a. Angle control card FØRMAT (I1)

Column 1 = 1 if the input angles are to be reported.

Column 1 = 0 or blank, if this output is not desired.

b. Reflection angles and identification. FØRMAT (2(A6, 2F8.3))

Two reflections are placed on each card. For a definition of the reference system used in measuring the angles, see the discussion of the subroutine.

col.	
1-6	6 BCD characters to identify the following reflection
7-14	θ, the Bragg angle
15-22	χ, the interplanar angle
23-28	6 BCD characters to identify the following reflection
29-36	θ, the Bragg angle
37-44	χ, the interplanar angle

Angles are given in degrees. The list of reflections is terminated with six zeros in the identification field following the last χ.

6. Input for ANGLE routine A2. (Used with three-dimensional orienter).

a. Angle control card FØRMAT(I1)

Column 1 = 1 if the input angles are to be reported.

Column 1 = 0 or blank if this output is not desired.

b. Reflection angles and identification FØRMAT (2(A6, 3F8.3))

Two reflections are placed on each card. For a definition of the reference system used in measuring the angles, see the discussion of the subroutine.

col.		
1-6	6 BCD characters identifying the following reflection.	
7-14	θ, the Bragg angle	
15-22	χ	orienter angles
23-30	ϕ	orienter angles
31-36	6 BCD characters identifying the following reflection.	
37-44	θ, the Bragg angle	
45-52	χ	orienter angles
53-60	ϕ	orienter angles

Angles are given in degrees. The list of reflections is terminated with six zeros in the identification field following the last ϕ.

CARD DECK FOR OAK RIDGE INSTALLATION

1. Monitor control cards
2. Program deck
3. Data
   a. Title card
   b. Control card
   c. Absorption coefficients
   d. Input for FACE routine
   e. Input for ANGLE routine
4. Repeat (3) if absorption coefficients are to be calculated for more than one crystal in a single monitor job.

OPERATING PROCEDURE FOR OAK RIDGE INSTALLATION

When preparing the monitor control cards the user should call for tapes on units 2 and 6. If either ANGLE routines A1 or A2 are used and the angle output is called for, the number of the files on tape 6 to be printed is equal to the number of crystals run. If the angle output has not been called for, there will be nothing on tape 6. The program rewinds tape 6 regardless of which ANGLE routine is being used.

SYMBOLS USED

EPS	input parameter. It is used in the calculation of ϵ, the tolerance used in the determination of the corners.
NS	amount of core storage available in data block.
NP	NP * M * (N+1) words are written in each block of magnetic tape in the first part of the program.
NANGL	number of reflections to be processed at one time.
N	number of planes bounding crystal.
V	volume of crystal.

V1	volume of crystal computed with weights read from magnetic tape; used as a check.
IDENT	BCD array containing crystal identification.
IT1	clock time at beginning of program; time for part I.
IT2	clock time at end of part I of program; time for part II.
IT3	clock time at end of program.
NANGL1	total number of reflections processed.
NMU	number of values of μ to be used.
NCØF	DATA subscript of first coefficient a_1 of planes describing crystal.
NEND	DATA subscript of last coefficient d_N of planes describing crystal.
NUM	DATA subscript of first numerator of $r_{\alpha s}$ in core.
NUMED	DATA subscript of last numerator of $r_{\alpha s}$ in core.
JCØR	the number of words to be reported in one line crystal corner output.
IANG	DATA subscript of first angle identification.
ISUM	DATA subscript of first absorption correction factor.
IDIF1	DATA subscript of the first of the N differences $d_s - a_s x_i$ (Part 1); DATA subscript of the first of the N denominators $a\gamma_{\alpha s} + b\gamma_{\alpha s} + c\gamma_{\alpha s}$ (Part 2).
IDIF2	DATA subscript of the first of the N differences $d_s - a_s x_i - b_s y_j$ (Part 1); DATA subscript of the first of the N denominators $a\gamma_{\beta s} + b\gamma_{\beta s} + c\gamma_{\beta s}$ (Part 2).
T	temporary storage used by Gaussian elimination routine.
TA	current value of $r_{\alpha s}$.
TB	current value of $r_{\beta s}$.
X	current value of x coordinate of point of integration.
RA	r_α
RB	r_β
WX	$(b-a)\ x_i$

Y	current value of y coordinate of point of integration.
WY	$(c-d)\ (a-b)\ x_i y_j$
Z	equivalent to I6, current value of z coordinate of point of integration.
A	a, lower limit of integration on x axis.
B	b, upper limit of integration on x axis.
DIF1	b-a; equivalent to B.
C	$c(x_i)$, lower limit of integration on y axis.
D	$d(x_i)$, upper limit of integration on y axis.
DIF2	$d(x_i) - c(x_i)$, equivalent to D.
E	$e(x_i, y_j)$ lower limit of integration on z axis.
F	$f(x_i, y_j)$ upper limit of integration on z axis.
VMU	equivalent to DATA; storage for values of μ.
DATA	name of block of storage which contains coefficients of faces, direction cosines of angles, values of $d_s - a_s x_i - b_s y_j - c_s z_k$, etc. The subscripts for each block are calculated.
NDATA	equivalent to DATA; fixed point name for DATA.
IX	DATA subscript for first index of corners of crystal.
R	Gaussian weights.
U	Gaussian points.
IP	
IQ	DATA subscripts used in determining corners of crystal.
IR	
I	IP1 and IQ1
I1, I2, I3, I4, I5, I6, I7, J, K, K1	Dummy subscripts for DATA.
EPS1	tolerance ϵ used in determining corners of crystal.
KØ	output option on the reporting of the corners of the crystal.
M	number of Gaussian points used in integration.

KØNST number of words of CØMMØN storage used excepting DATA block.

NP1 number of blocks on magnetic tape.

STORAGE TABLE FOR THE ARRAY DATA*

Number of words		Subscript
NMU ≤ 6	$\mu_1, \ldots, \mu_{NMU}$	1 | NMU
4 * N	$a_s, b_s, c_s, d_s, (s = 1, \ldots, n)$	NCØF | NEND
NP*M*(N+1)	$d_s - a_s x_i - b_s y_j - c_s z_k$ $(b-a)(d-c)(f-e)R_i R_j R_k$ for $s = 1, \ldots, n$ $i, j, k = 1, \ldots, m$	NUM | NUMED
N	(Part 1) $d_s - a_s x_i$ $(s = 1, \ldots, n)$ (Part 2) $a_s \gamma_{\alpha x} + b_s \gamma_{\alpha y} + c_s \gamma_{\alpha z}$	IDIF1 | IDIF2-1
N	(Part 1) $d_s - a_s x_i - b_s y_j$ $(s = 1, \ldots, n)$ (Part 2) $a_s \gamma_{\beta x} + b_s \gamma_{\beta y} + c_x \gamma_{\beta z}$	IDIF2 | IX-1
12	(Part 1) Indices of planes and coordinates of corners	IX | IX+11
7*NANGL	(Part 2) Id, $\gamma_{\alpha x}, \gamma_{\alpha y}, \gamma_{\alpha z}, \gamma_{\beta x}, \gamma_{\beta y}, \gamma_{\beta z}$ for each reflection	IANG | ISUM-1
NMU*NANGL	(Part 2) $A_1(\mu_k), A_2(\mu_k) \ldots$	ISUM |

*DATA is equivalent to VMU and NDATA.

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C        ABSORPTION CALCULATION,  3-DIMENSIONAL                          P1   000
      COMMON EPS,NS,NB,NP,NANGL,N,V,V1,IDENT,IT1,IT2,IT3,NANGL1,NMU,     P1   001
     2NCOF,NEND,NUM,NUMED,IDIF1,IDIF2,IANG,ISUM,JCOR,                    P1   002
     3T,X,WX,Y,WY,Z,A,B,C,D,E,F,DIF1,DIF2,DIF3,TA,TB,RA,RB,              P1   003
     4VMU,DATA                                                           P1   004
      DIMENSIONIDENT(12),T(12),R(16),U(16),VMU(1),DATA(1),NDATA(1)       P1   005
      EQUIVALENCE(EPS,DUM4),(NS,DUM5),                                   P1   006
     1(NB,DUM6),(NP,DUM7),(NANGL,DUM8),(N,DUM9),(V,DUM10),(V1,DUM11),    P1   007
     2(IDENT,DUM12),(IT1,DUM13),(IT2,DUM14),(IT3,DUM15),(NANGL1,DUM16),  P1   008
     3(NMU,DUM17),(IANG,DU33),(ISUM,DU34),                               P1   009
     4(NCOF,DUM19),(NEND,DUM20),(NUM,DUM21),(NUMED,DUM22),(JCOR,DUM23),  P1   010
     5(IDIF1,DU31),(IDIF2,DU32),(T(3),X),(T(6),WX),(T(9),Y),(T(12),WY),  P1   011
     6(Z,I6),(A,DUM24),(B,DIF1),(C,DUM25),(D,DIF2),(E,DUM26),(F,DIF3),   P1   012
     7(IP1,IQ1,I),(T(1),TA),(T(2),TB),(T(4),RA),(T(5),RB),               P1   013
     8(DATA,VMU,NDATA)                                                   P1   014
      READINPUTTAPE10,1003,M                                             P1   015
      IF(M-16)9001,9001,9002                                             P1   016
 9001 READINPUTTAPE10,1005,(U(I),I=1,M),(R(I),I=1,M)                     P1   017
      REWIND 6                                                           P1   018
      LINES =50                                                          P1   019
      SENSELIGHT0                                                        P1   020
      CALLSIZE(NS)                                                       P1   021
 3213 CALLCLOCK(IT1,DATE)                                                P1   022
      READINPUTTAPE10,1001,(IDENT(I),I=1,12)                             P1   023
      READINPUTTAPE10,1003,NMU,EPS,KO                                    P1   024
      IF(NMU-6)314,314,315                                               P1   025
  314 NCOF=NMU+1                                                         P1   026
      READINPUTTAPE10,1004,(VMU(I),I=1,NMU)                              P1   027
      CALLFACE(IDENT,N,DATA,NCOF,DATE)                                   P1   028
 9020 CALLEPSR(EPS,EPS1)                                                 P1   029
      I1=NS-KONST-NMU-6*N-12                                             P1   030
      NP=I1/(M*(N+1))                                                    P1   031
      I2=M**2                                                            P1   032
  316 IF(XMODF(I2,NP))318,312,318                                        P1   033
  318 NP=NP-1                                                            P1   034
      GO TO316                                                           P1   035
  312 IF(NP)8313,8313,311                                                P1   036
  311 NANGL=(I1-NP*M*(N+1)+12)/(7+NMU)                                   P1   037
      IF(NANGL-2)317,317,313                                             P1   038
  317 IF(NP-1)8313,8313,318                                              P1   039
  313 NB=I2/NP                                                           P1   040
      NEND=NCOF+4*N-1                                                    P1   041
```

```
      NUM=NEND+1                                                        P1   042
      NUMED=NP*M*(N+1)+NEND                                             P1   043
      IDIF1=NUMED+1                                                     P1   044
      IDIF2=IDIF1+N                                                     P1   045
      IX=IDIF2+N                                                        P1   046
      IANG=IX                                                           P1   047
      ISUM=NANGL*7+IANG                                                 P1   048
C        DETERMINE COEFFICIENTS OF CORNERS AND REPORT                   P1   049
C        CALCULATE A, B, B-A                                            P1   050
      IF(NB-1)7006,7006,7007                                            P1   051
 7007 REWIND2                                                           P1   052
 7006 IF(KO)60,60,61                                                    P1   053
   61 CALLIDOUT(IDENT,DATE,9)                                           P1   054
      WRITEOUTPUTTAPE 9,2001                                            P1   055
      NLINES=LINES                                                      P1   056
   60 A=10.0E37                                                         P1   057
      B=-A                                                              P1   058
      JCOR=0                                                            P1   059
      I1=N-2                                                            P1   060
      DO27IP=1,I1                                                       P1   061
      IP1=IP+1                                                          P1   062
      I1=N-1                                                            P1   063
      DO26IQ=IP1,I1                                                     P1   064
      IQ1=IQ+1                                                          P1   065
      DO54IR=IQ1,N                                                      P1   066
      I1=NCOF+4*(IP-1)                                                  P1   067
      DO24K=1,12,3                                                      P1   068
      T(K)=DATA(I1)                                                     P1   069
   24 I1=I1+1                                                           P1   070
      I1=NCOF+4*(IQ-1)                                                  P1   071
      DO23K=1,12,3                                                      P1   072
      T(K+1)=DATA(I1)                                                   P1   073
   23 I1=I1+1                                                           P1   074
      I1=NCOF+4*(IR-1)                                                  P1   075
      DO22K=1,12,3                                                      P1   076
      T(K+2)=DATA(I1)                                                   P1   077
   22 I1=I1+1                                                           P1   078
      CALLGAUSOL(T,3)                                                   P1   079
      IF(SENSELIGHT2)54,69                                              P1   080
   69 DO28K=NCOF,NEND,4                                                 P1   081
      IF(DATA(K)*T(10)+DATA(K+1)*T(11)+DATA(K+2)*T(12)-DATA(K+3)+EPS1)5 P1   082
     14,28,28                                                           P1   083
   28 CONTINUE                                                          P1   084
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```
      IF(A-T(10))50,50,51                                               P1   085
   51 A=T(10)                                                           P1   086
   50 IF(T(10)-B)52,52,53                                               P1   087
   53 B=T(10)                                                           P1   088
   52 IF(KO)54,54,62                                                    P1   089
   62 I1=IX+JCOR                                                        P1   090
      NDATA(I1)=IP                                                      P1   091
      NDATA(I1+1)=IQ                                                    P1   092
      NDATA(I1+2)=IR                                                    P1   093
      DO20K=3,5                                                         P1   094
      I1=JCOR+K+IX                                                      P1   095
   20 DATA(I1)=T(K+7)                                                   P1   096
      JCOR=JCOR+6                                                       P1   097
      IF(JCOR-12)54,29,29                                               P1   098
   29 CALLOCOR(DATA,IX,JCOR)                                            P1   099
   54 CONTINUE                                                          P1   100
   26 CONTINUE                                                          P1   101
   27 CONTINUE                                                          P1   102
      IF(KO)57,57,64                                                    P1   103
   64 IF(JCOR)57,57,58                                                  P1   104
   58 CALLOCOR(DATA,IX,JCOR)                                            P1   105
   57 DIF1=B-A                                                          P1   106
      IF(DIF1)56,56,55                                                  P1   107
   55 CONTINUE                                                          P1   108
      V =0.0                                                            P1   109
      NP1=NP                                                            P1   110
      K1=NUM                                                            P1   111
      DO107I=1,M                                                        P1   112
      X=A+DIF1*U(I)                                                     P1   113
      WX=R(I)*DIF1                                                      P1   114
      I2=IDIF1                                                          P1   115
      DO70I1=NCOF,NEND,4                                                P1   116
      DATA(I2)=DATA(I1+3)-DATA(I1)*X                                    P1   117
   70 I2=I2+1                                                           P1   118
C        CALCULATE C, D, D-C                                            P1   119
      C=10.0E37                                                         P1   120
      D=-C                                                              P1   121
      I20=N-1                                                           P1   122
      DO71IP=1,I20                                                      P1   123
      IP1=IP+1                                                          P1   124
      DO76IQ=IP1,N                                                      P1   125
      I1=NCOF+1+4*(IP-1)                                                P1   126
```

```
      DO73K=1,4,3                                                       P1   127
      T(K)=DATA(I1)                                                     P1   128
   73 I1=I1+1                                                           P1   129
      I1=NCOF+1+4*(IQ-1)                                                P1   130
      DO74K=1,4,3                                                       P1   131
      T(K+1)=DATA(I1)                                                   P1   132
   74 I1=I1+1                                                           P1   133
      I1=IDIF1+IP-1                                                     P1   134
      T(7)=DATA(I1)                                                     P1   135
      I1=IDIF1+IQ-1                                                     P1   136
      T(8)=DATA(I1)                                                     P1   137
      CALLGAUSOL(T,2)                                                   P1   138
      IF(SENSELIGHT2)76,68                                              P1   139
   68 I2=IDIF1                                                          P1   140
      DO75I1=NCOF,NEND,4                                                P1   141
      IF(DATA(I1+1)*T(7)+DATA(I1+2)*T(8)-DATA(I2)+EPS1)76,75,75         P1   142
   75 I2=I2+1                                                           P1   143
      IF(C-T(7))77,77,78                                                P1   144
   78 C=T(7)                                                            P1   145
   77 IF(T(7)-D)76,76,79                                                P1   146
   79 D=T(7)                                                            P1   147
   76 CONTINUE                                                          P1   148
   71 CONTINUE                                                          P1   149
      DIF2=D-C                                                          P1   150
      IF(DIF2)72,72,80                                                  P1   151
   80 CONTINUE                                                          P1   152
      DO91J=1,M                                                         P1   153
      Y=C+DIF2*U(J)                                                     P1   154
      WY=WX*DIF2*R(J)                                                   P1   155
      I2=IDIF1                                                          P1   156
      I3=IDIF2                                                          P1   157
      DO90I1=NCOF,NEND,4                                                P1   158
      DATA(I3)=DATA(I2)-DATA(I1+1)*Y                                    P1   159
      I2=I2+1                                                           P1   160
   90 I3=I3+1                                                           P1   161
      E=10.0E37                                                         P1   162
      F=-E                                                              P1   163
      I3=IDIF2                                                          P1   164
      DO93I1=NCOF,NEND,4                                                P1   165
      Z=DATA(I3)/DATA(I1+2)                                             P1   166
      I4=IDIF2                                                          P1   167
      DO94I2=NCOF,NEND,4                                                P1   168
      IF(DATA(I2+2)*Z-DATA(I4)+EPS1)93,94,94                            P1   169
```

```
   94 I4=I4+1                                                          P1   170
      IF(E-Z)96,96,97                                                  P1   171
   97 E=Z                                                              P1   172
   96 IF(Z-F)93,93,98                                                  P1   173
   98 F=Z                                                              P1   174
   93 I3=I3+1                                                          P1   175
      DIF3=F-E                                                         P1   176
      IF(DIF3)99,99,100                                                P1   177
  100 CONTINUE                                                         P1   178
      DO101K=1,M                                                       P1   179
      Z=E+DIF3*U(K)                                                    P1   180
      I2=IDIF2                                                         P1   181
      DO102I1=NCOF,NEND,4                                              P1   182
      DATA(K1)=DATA(I2)-DATA(I1+2)*Z                                   P1   183
      IF(DATA(K1))103,103,104                                          P1   184
  104 DATA(K1)=0.0                                                     P1   185
  103 K1=K1+1                                                          P1   186
  102 I2=I2+1                                                          P1   187
      DATA(K1)=WY*DIF3*R(K)                                            P1   188
      V=V+DATA(K1)                                                     P1   189
  101 K1=K1+1                                                          P1   190
      IF(NB-1)91,91,7002                                               P1   191
 7002 NP1=NP1-1                                                        P1   192
      IF(NP1)105,105,91                                                P1   193
  105 WRITETAPE2,(DATA(I1),I1=NUM,NUMED)                               P1   194
      K1=NUM                                                           P1   195
      NP1=NP                                                           P1   196
   91 CONTINUE                                                         P1   197
  107 CONTINUE                                                         P1   198
      IF(NB-1)7004,7004,7005                                           P1   199
 7005 ENDFILE2                                                         P1   200
      REWIND2                                                          P1   201
 7004 CALLCLOCK(IT2,DATE)                                              P1   202
C     END OF PART I,  BEGINNING OF PART II                             P1   204
      CALLIDOUT(IDENT,DATE,9)                                          P1   205
      WRITEOUTPUTTAPE9,2003,(VMU(I),I=1,NMU)                           P1   206
      NANGL1=0                                                         P1   207
  211 CALLANGLE(IDENT,DATA,IANG,NANGL,DATE,NANGL1)                     P1   208
      V1=0.0                                                           P1   209
      NANGL1=NANGL1+NANGL                                              P1   210
      K1 =N+1                                                          P1   211
      I3=NANGL*7-1+IANG                                                P1   212
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```
      I2=ISUM+NMU*NANGL-1                                               P1   213
      DO200I1=ISUM,I2                                                   P1   214
  200 DATA(I1)=0.0                                                      P1   215
      DO201I1=1,NB                                                      P1   216
      IF(NB-1)7001,7001,7003                                            P1   217
 7003 READTAPE2,(DATA(I2),I2=NUM,NUMED)                                 P1   218
 7001 I6=ISUM                                                           P1   219
      DO202I2=IANG,I3,7                                                 P1   220
      I9=IDIF1                                                          P1   221
      I8=IDIF2                                                          P1   222
      DO203I4=NCOF,NEND,4                                               P1   223
      DATA(I9)=DATA(I4)*DATA(I2+1)+DATA(I4+1)*DATA(I2+2)+DATA(I4+2)*DATAP1   224
     1(I2+3)                                                            P1   225
      DATA(I8)=DATA(I4)*DATA(I2+4)+DATA(I4+1)*DATA(I2+5)+DATA(I4+2)*DATAP1   226
     1(I2+6)                                                            P1   227
      I9=I9+1                                                           P1   228
  203 I8=I8+1                                                           P1   229
      DO215I7=NUM,NUMED,K1                                              P1   230
      I5=I7                                                             P1   231
      RA=10.0E37                                                        P1   232
      RB=RA                                                             P1   233
      I9=IDIF2-1                                                        P1   234
      I8=IDIF2                                                          P1   235
      DO208I4=IDIF1,I9                                                  P1   236
      IF(DATA(I4))911,213,213                                           P1   237
  911 TA=DATA(I5)/DATA(I4)                                              P1   238
      IF(RA-TA)213,213,205                                              P1   239
  205 RA=TA                                                             P1   240
  213 IF(DATA(I8))216,217,217                                           P1   241
  216 TB=DATA(I5)/DATA(I8)                                              P1   242
      IF(RB-TB)217,217,207                                              P1   243
  207 RB=TB                                                             P1   244
  217 I5=I5+1                                                           P1   245
      I8=I8+1                                                           P1   246
  208 CONTINUE                                                          P1   247
      RA=RA+RB                                                          P1   248
      I10=I6                                                            P1   249
      DO206I4=1,NMU                                                     P1   250
      DATA(I10)=DATA(I10)+EXPF(-VMU(I4)*RA)*DATA(I5)                    P1   251
  206 I10=I10+1                                                         P1   252
  215 CONTINUE                                                          P1   253
      I6=I6+NMU                                                         P1   254
  202 CONTINUE                                                          P1   255
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      DO8204I4=NUM,NUMED,K1                                             P1   256
      I5=I4+N                                                           P1   257
 8204 V1=V1+DATA(I5)                                                    P1   258
  201 CONTINUE                                                          P1   259
      IF(NB-1)7009,7009,7010                                            P1   260
 7010 REWIND2                                                           P1   261
 7009 I6=ISUM+NANGL*NMU-1                                               P1   262
      DO8021I4=ISUM,I6                                                  P1   263
 8021 DATA(I4)=DATA(I4)/V                                               P1   264
      IF(V-V1)209,210,209                                               P1   265
  210 I2=ISUM                                                           P1   266
      I5=IANG+7*NANGL-1                                                 P1   267
      DO400I1=IANG,I5,7                                                 P1   268
      I3=I2+NMU-1                                                       P1   269
      NLINES=NLINES-1                                                   P1   270
      IF(NLINES)240,240,241                                             P1   271
  240 NLINES=LINES                                                      P1   272
      CALLIDOUT(IDENT,DATE,9)                                           P1   273
      WRITEOUTPUTTAPE9,2003,(VMU(I),I=1,NMU)                            P1   274
  241 WRITE OUTPUT TAPE9,2008,DATA(I1),(DATA(I4),I4=I2,I3)              P1   275
  400 I2=I3+1                                                           P1   276
      IF(SENSELIGHT1)212,211                                            P1   277
  212 CALLCLOCK(IT3,DATE)                                               P1   278
      IT1=IT2-IT1                                                       P1   279
      IT2=IT3-IT2                                                       P1   280
      CALLIDOUT(IDENT,DATE,9)                                           P1   281
      WRITEOUTPUTTAPE9,2093,V                                           P1   282
      WRITEOUTPUTTAPE9,2004,N,NANGL1,NMU,IT1,IT2                        P1   283
      GOTO8213                                                          P1   284
C     ERROR RETURNS                                                     P1   285
  315 CALLIDOUT(IDENT,DATE,9)                                           P1   286
      WRITEOUTPUTTAPE9,2010,NMU                                         P1   287
      CALLEXIT                                                          P1   288
   56 CALLIDOUT(IDENT,DATE,9)                                           P1   289
      WRITEOUTPUTTAPE9,2011,A,DIF1                                      P1   290
      CALLERROR                                                         P1   291
   72 CALLIDOUT(IDENT,DATE,9)                                           P1   292
      WRITEOUTPUTTAPE9,2012,C,DIF2                                      P1   293
      CALLERROR                                                         P1   294
   99 CALLIDOUT(IDENT,DATE,9)                                           P1   295
      WRITEOUTPUTTAPE9,2013,E,DIF3                                      P1   296
      CALLERROR                                                         P1   297
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 209 CALLIDOUT(IDENT,DATE,9)                                            P1   298
     WRITE OUTPUTTAPE9,2020,V,V1                                        P1   299
     CALL ERROR                                                         P1   300
9021 CALLIDOUT(IDENT,DATE,9)                                            P1   301
     WRITEOUTPUTTAPE9,2092,N                                            P1   302
     CALLEXIT                                                           P1   303
9002 WRITEOUTPUTTAPE9,2090,M                                            P1   304
     CALLEXIT                                                           P1   305
3313 CALLIDOUT(IDENT,DATE,9)                                            P1   306
     WRITEOUTPUTTAPE9,2313,N,M,NMU,NS,NP                                P1   307
     CALLEXIT                                                           P1   308
2313 FORMAT(36H0MEMORY IS TOO SMALL FOR PARAMETERS./4H0N =I3,3HM =I3,5HP1   309
    1NMU =I2,19HAVAILABLE STORAGE =I6,4HNP =I5)                         P1   310
2090 FORMAT(21H1M IS TOO LARGE.  M = I5)                                P1   311
2092 FORMAT(5H0N = I5,15H  IS TOO LARGE.)                               P1   312
2093 FORMAT(10H0VOLUME = F15.8)                                         P1   313
1001 FORMAT(12A6)                                                       P1   314
1002 FORMAT(1I1)                                                        P1   315
1003 FORMAT(I5,E15.8,I5)                                                P1   316
1004 FORMAT(6E10.8)                                                     P1   317
1005 FORMAT(4F10.8)                                                     P1   318
2001 FORMAT(34H0COORDINATES OF CORNERS OF CRYSTAL/52H0INDEX OF PLANES FP1   319
    1ORMING CORNER, FOLLOWED BY X, Y, Z//)                              P1   320
2003 FORMAT(33H0ABSORPTION CORRECTION FACTOR,  A/6H0MU = 6(E10.5)//)    P1   321
2004 FORMAT(5H0N = I5,3X,19HNUMBER OF ANGLES = I5,3X,15HNUMBER OF MU = P1   322
    1I2//29H TIME USED IN PARTS 1 AND 2 = 2I10,3X,18HIN 10S OF SECONDS.P1   323
    2)                                                                  P1   324
2008 FORMAT(1H01A6,3X,6F12.8)                                           P1   325
2010 FORMAT(29H0INPUT ERROR.  NUMBER OF MU =I5,24HWHICH IS GREATER THANP1   326
    1 6.)                                                               P1   327
2011 FORMAT(62H0ERROR IN CALCULATION OF UPPER AND LOWER LIMITS (B, A,).P1   328
    1  A = E15.8,8H, B-A = E15.8/19H0CORE DUMPS FOLLOW.)                P1   329
2012 FORMAT(62H0ERROR IN CALCULATION OF UPPER AND LOWER LIMITS (D, C). P1   330
    1  C = E15.8,8H, D-C = E15.8/19H0CORE DUMPS FOLLOW.)                P1   331
2013 FORMAT(62H0ERROR IN CALCULATION OF UPPER AND LOWER LIMITS (F, E). P1   332
    1  E = E15.8,8H, F-E = E15.8/19H0CORE DUMPS FOLLOW.)                P1   333
2020 FORMAT(58H0ERROR.  VOLUME FROM CORE IS NOT EQUAL TO VOLUME FROM TAP1   334
    1PE/11H0V(CORE) = E15.8,10HV(TAPE) = E15.8/14H0DUMP FOLLOWS.)       P1   335
     END (0,1,0,0,0)                                                    P1   336
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```
C        SUBROUTINE GAUSOL(A,N)                                          G   337
      SUBROUTINE GAUSOL(A,N)                                             G   338
      DIMENSION A(3,4)                                                   G   339
C        SOLUTION OF SYSTEM OF EQUATIONS BY GAUSSIAN ELIMINATION         G   340
C             USING INTERCHANGES                                         G   341
C             A = NAME OF MATRIX (ORIGINAL MATRIX IS DESTROYED)          G   342
C                 MATRIX IS STORED BY COLUMNS, VECTOR FOLLOWS            G   343
C             N = ORDER OF MATRIX                                        G   344
C                 (N MUST BE LESS THAN OR EQUAL DIMENSION STATEMENT)     G   345
C        SOLUTION IS FOUND IN A(1,N+1) THROUGH A(N,N+1)                  G   346
      IF(SENSELIGHT2)20,20                                               G   347
 20   N2=N-1                                                             G   348
      N1=N+1                                                             G   349
      DO9I1=1,N2                                                         G   350
      L=0                                                                G   351
      R=A(I1,I1)                                                         G   352
      I11=I1+1                                                           G   353
      DO2IR=I11,N                                                        G   354
      IF(ABSF(R)-ABSF(A(IR,I1)))3,2,2                                    G   355
    3 R=A(IR,I1)                                                         G   356
      L=IR                                                               G   357
    2 CONTINUE                                                           G   358
      IF(L)4,4,5                                                         G   359
    5 DO6IJ=I1,N1                                                        G   360
      X=A(L,IJ)                                                          G   361
      A(L,IJ)=A(I1,IJ)                                                   G   362
    6 A(I1,IJ)=X                                                         G   363
    4 DO8I2=I11,N                                                        G   364
      T=A(I2,I1)/A(I1,I1)                                                G   365
      DO7I3=I11,N1                                                       G   366
    7 A(I2,I3)=A(I2,I3)-A(I1,I3)*T                                       G   367
    8 CONTINUE                                                           G   368
    9 CONTINUE                                                           G   369
      A(N,N1)=A(N,N1)/A(N,N)                                             G   370
      DO11I=1,N2                                                         G   371
      I1=N-I                                                             G   372
      I2=I1+1                                                            G   373
      DO10I3=I2,N                                                        G   374
   10 A(I1,N1)=A(I1,N1)-A(I1,I3)*A(I3,N1)                                G   375
   11 A(I1,N1)=A(I1,N1)/A(I1,I1)                                         G   376
      IFDIVIDECHECK15,14                                                 G   377
   15 SENSELIGHT2                                                        G   378
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   14 IF ACCUMULATOR OVERFLOW12,17                                    G   379
   12 SENSELIGHT2                                                     G   380
   17 IFQUOTIENTOVERFLOW16,13                                         G   381
   16 SENSELIGHT2                                                     G   382
   13 RETURN                                                          G   383
      END(0,1,0,0,1)                                                  G   384


C        REPORT CRYSTAL IDENTIFICATION                               ID   385
      SUBROUTINE IDOUT(IDENT,DATE,N)                                 ID   386
      DIMENSION IDENT(12)                                            ID   387
      WRITEOUTPUTTAPEN,2001,(IDENT(I),I=1,12),DATE                   ID   388
 2001 FORMAT(1H112A6,41X,1A6)                                        ID   389
      RETURN                                                         ID   390
      END(0,1,0,0,0)                                                 ID   391


C        REPORT ONE LINE OF ONE OR TWO CORNERS OF A CRYSTAL          OC   392
C           FOR 3-DIMENSIONAL PROBLEM                                OC   393
C        FIRST THREE NUMBERS REPORTED ARE INTEGERS WHICH DESIGNATE   OC   394
C           THE PLANES WHICH FORM CORNERS,                           OC   395
C        SECOND THREE NUMBERS ARE THE X, Y, Z COORDINATES OF THE CORNER.OC   396
C        NOTATION  X = LOCATION OF ARRAY OF 12 NUMBERS               OC   397
C                 IX = SUBSCRIPT OF FIRST NUMBER OF ARRAY X          OC   398
C               JCOR = 6*I, WHERE I IS THE NUMBER OF CORNERS TO REPORT OC   399
      SUBROUTINEOCOR(X,IX,JCOR)                                      OC   400
      DIMENSION X(1)                                                 OC   401
      JCOR =JCOR+IX-1                                                OC   402
      WRITE OUTPUT TAPE9,2002,(X(K),K=IX,JCOR)                       OC   403
      JCOR=0                                                         OC   404
 2002 FORMAT(1H 2(3I3.0,3F13.9,4X))                                  OC   405
      RETURN                                                         OC   406
      END(0,1,0,0,0)                                                 OC   407


C           DUMMY EPSR SUBROUTINE                                    E1   408
C        TO CALCULATE EPS1 = TOLERANCE FOR CORNERS OF CRYSTAL        E1   409
      SUBROUTINEEPSR(EPS,EPS1)                                       E1   410
      EPS1=EPS                                                       E1   411
      RETURN                                                         E1   412
      END(0,1,0,1,0)                                                 E1   413
```

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C       DUMMY CLOCK SUBROUTINE                                          C1   414
C       PLACES 0 IN TIME, BLANKS IN DATE                                C1   415
       SUBROUTINE CLOCK(IT,DATE)                                        C1   416
S BLK  ALF                                                              C1   417
       IT =0                                                            C1   418
       DATE=BLK                                                         C1   419
       RETURN                                                           C1   420
       END(0,1,0,0,0)                                                   C1   421

*        CLOCK SUBROUTINE                                               C2   422
        FUL                     PROGRAM CARD                            C2   423
        ORG 0                   PROGRAM CARD                            C2   424
        MZE 0,0,4               9L                                      C2   425
        PZE 0                   9R                                      C2   426
        PZE T+1                 8L                                      C2   427
        PZE 0                   8R                                      C2   428
        BCD 1CLOCK              7L                                      C2   429
        PZE 0                   7R                                      C2   430
        ORG 0                                                           C2   431
        REL                                                             C2   432
        CLA 1,4                                                         C2   433
        STA ADD                                                         C2   434
        CLA 2,4                                                         C2   435
        STA ADD+2                                                       C2   436
        SXD T,4                                                         C2   437
        TSX CLOCK,4                                                     C2   438
        HTR *+1                                                         C2   439
        ALS 18                                                          C2   440
 ADD    STO 0                                                           C2   441
        CLA DATE                                                        C2   442
        STO 0                                                           C2   443
        LXD T,4                                                         C2   444
        TRA 3,4                                                         C2   445
 DATE   BSS 1                                                           C2   446
ORCLK5  REM                                                             C2   447
        REM READ CHRONO-LOG CLOCK ROUTINE.  ERROR RETURN IF CLOCK FAILS C2   448
        REM BINARY TIME (10 SEC.=1 UNIT) IN AC. FOR USE WITH CHRONO-LOG C2   449
        REM DIGITAL CLOCK MODEL 2704-1 WIRED TO 716 PRINT ECHO ENTRIES. C2   450
 CLOCK  RPR                                                             C2   451
        SPR 6                   SENSE THE CLOCK                         C2   452
        STZ DATE                                                        C2   453
```

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```
        SXD *+35,2                                                      C2   454
        STZ COMMON                                                      C2   455
        SXD COMMON+1,1                                                  C2   456
        LXD *+13,1                                                      C2   457
        TNX *+15,1,2                                                    C2   458
        CPY DATE                                                        C2   459
        CPY COMMON                                                      C2   460
        TQP *-3                                                         C2   461
        LXD *+15,2                                                      C2   462
        LXA *+1,1                                                       C2   463
        PXD 3                                                           C2   464
        RQL 1                                                           C2   465
        TQP *+5                                                         C2   466
        RQL 1                                                           C2   467
        TNX *+6,1,1                                                     C2   468
        TQP *-2                ERROR IF MQ MINUS                        C2   469
        TXL *+3,,47                                                     C2   470
        ADD *+14,2                                                      C2   471
        TIX *-7,1,1                                                     C2   472
        TXI *+12,4,1           ERROR RETURN                             C2   473
        TNX *+11,2,1                                                    C2   474
        TRA *+5,2                                                       C2   475
        TXI *-10,1,9                                                    C2   476
        TXI *-11,1,5                                                    C2   477
        TXI *-12,1,9                                                    C2   478
        TXI *-13,1,5                                                    C2   479
        DEC 3600,360,60,6,1                                             C2   480
        LXD COMMON+1,1                                                  C2   481
        LXD *+3,2                                                       C2   482
        SPT                                                             C2   483
        TRA 2,4                                                         C2   484
        TXL *-2                                                         C2   485
COMMON  BSS 2                                                           C2   486
 T      HTR 0                                                           C2   487
        END 0                                                           C2   488

C         SUBROUTINE ANGLE (IDENT,DATA,IANG,NANGL,DATE,NANGL1)          A1   489
C         USING ONLY TWO ANGLES, THETA AND CHI                          A1   490
C         ZERO IS STORED FOR REMAINING DIRECTION COSINES                A1   491
      SUBROUTINEANGLE(IDENT,DATA,IANG,NANGL,DATE,NANGL1)                A1   492
      DIMENSIONIDENT(12),DATA(1)                                        A1   493
      K1=0                                                              A1   494
```

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```
      I3=IANG+7*NANGL-1                                                 A1   495
      IF(NANGL1)30,31,30                                                A1   496
   31 READINPUTTAPE10,1002,NOP                                          A1   497
   30 DO10I2=IANG,I3,14                                                 A1   498
      I4=I2+13                                                          A1   499
      READINPUTTAPE10,1001,(DATA(I1),DATA(I1+1),DATA(I1+2),I1=I2,I4,7)  A1   500
      DO13I5=I2,I4,7                                                    A1   501
      IF(DATA(I5)) 13,12,13                                             A1   502
   13 K1=K1+1                                                           A1   503
      IF(NANGL-K1-2) 11,10,10                                           A1   504
   12 SENSELIGHT1                                                       A1   505
      NANGL=K1                                                          A1   506
      GOTO11                                                            A1   507
   10 CONTINUE                                                          A1   508
   11 I3=IANG+7*NANGL-1                                                 A1   509
      IF(NOP)17,16,15                                                   A1   510
   15 NOP=-1                                                            A1   511
      CALLIDOUT(IDENT,DATE,6)                                           A1   512
      WRITEOUTPUTTAPE6,2001                                             A1   513
   17 WRITEOUTPUTTAPE6,2002,(DATA(I1),DATA(I1+1),DATA(I1+2),I1=IANG,I3,7A1   514
     1)                                                                 A1   515
       IF(SENSELIGHT1)20,16                                             A1   516
   20 SENSELIGHT1                                                       A1   517
       END FILE 6                                                       A1   518
   16 DO14I2=IANG,I3,7                                                  A1   519
      DATA(I2+6)=(DATA(I2+2)-DATA(I2+1))*0.0174533                      A1   520
      DATA(I2+3)=(DATA(I2+2)+DATA(I2+1))*0.0174533+3.1415926            A1   521
      DATA(I2+1)=COSF(DATA(I2+3))                                       A1   522
      DATA(I2+2)=SINF(DATA(I2+3))                                       A1   523
      DATA(I2+3)=0                                                      A1   524
      DATA(I2+4)=COSF(DATA(I2+6))                                       A1   525
      DATA(I2+5)=SINF(DATA(I2+6))                                       A1   526
   14 DATA(I2+6)=0                                                      A1   527
 1001 FORMAT(2(1A6,2F8.3))                                              A1   528
 1002 FORMAT(1I1)                                                       A1   529
 2001 FORMAT(12H0ANGLE INPUT/1H0,9X,14HTHETA       CHI//)               A1   530
 2002 FORMAT(1H (2(1A6,2F10.3,5X)))                                     A1   531
      RETURN                                                            A1   532
      END (0,1,0,0,0)                                                   A1   533
```

```
C        SUBROUTINE ANGLE(2),  FOR 3-D ORIENTING EQUIPMENT                A2   534
C     WRITTEN 9-9-60                                                      A2   535
      SUBROUTINEANGLE(IDENT,DATA,IANG,NANGL,DATE,NANGL1)                  A2   536
      DIMENSION IDENT(12),DATA(1)                                         A2   537
      K1#0                                                                A2   538
      I3#IANG+7*NANGL-1                                                   A2   539
      IF(NANGL1)30,31,30                                                  A2   540
   31 READINPUTTAPE10,1002,NOP                                            A2   541
   30 DO101I2#IANG,I3,14                                                  A2   542
      CONTINUE                                                            A2   543
      CONTINUE                                                            A2   544
      I4#I2+13                                                            A2   545
      READINPUTTAPE10,1001,(DATA(I1),DATA(I1+1),DATA(I1+2),DATA(I1%3)     A2   546
     1,I1#I2,I4,7)                                                        A2   547
      DO13I5#I2,I4,7                                                      A2   548
      IF(DATA(I5)) 13,12,13                                               A2   549
   13 K1#K1+1                                                             A2   550
      IF(NANGL-K1-2) 11,10,10                                             A2   551
   12 SENSELIGHT1                                                         A2   552
      NANGL#K1                                                            A2   553
      GOTO11                                                              A2   554
   10 CONTINUE                                                            A2   555
   11 I3#IANG+7*NANGL-1                                                   A2   556
      IF(NOP)17,16,15                                                     A2   557
   15 NOP#-1                                                              A2   558
      CALLIDOUT(IDENT,DATE,6)                                             A2   559
      WRITEOUTPUTTAPE6,2001                                               A2   560
   17 WRITEOUTPUTTAPE6,2002,(DATA(I1),DATA(I1+1),DATA(I1+2), DATA(I1+3),A2   561
     1I1#IANG,I3,7)                                                       A2   562
       IF(SENSELIGHT1)20,16                                               A2   563
   20 SENSELIGHT1                                                         A2   564
       END FILE 6                                                         A2   565
   16 DO14I2#IANG,I3,7                                                    A2   566
      DATA(I2+1)#DATA(I2+1)*0.174532925E-1                                A2   567
      DATA(I2+2)#DATA(I2+2)*0.174532925E-1                                A2   568
      DATA(I2+3)#DATA(I2+3)*0.174532925E-1                                A2   569
      T1#SINF(DATA(I2+1))                                                 A2   570
      T2#COSF(DATA(I2+1))                                                 A2   571
      T3#VINF(DATA(I2+3))                                                 A2   572
      T4#COSF(DATA(I2+3))                                                 A2   573
      DATA(I2+6)#SINF(DATA(I2+2))*T1                                      A2   574
      DATA(I2+3)#COSF(DATA(I2+2))*T1                                      A2   575
      DATA(I2+4)#DATA(I2+3)*T4                                            A2   576
```

```
      DATA(I2+5)=T3*T2                                                  A2   577
      DATA(I2+1)=DATA(I2+4)+DATA(I2+5)                                  A2   578
      DATA(I2+4)=DATA(I2+4)-DATA(I2+5)                                  A2   579
      DATA(I2+5)=T4*T2                                                  A2   580
      DATA(I2+3)=DATA(I2+3)*T3                                          A2   581
      DATA(I2+2)=DATA(I2+3)-DATA(I2+5)                                  A2   582
      DATA(I2+5)=DATA(I2+3)+DATA(I2+5)                                  A2   583
      DATA(I2+3)=DATA(I2+6)                                             A2   584
   14 CONTINUE                                                          A2   585
 1001 FORMAT(2(1A6,3F8.3))                                              A2   586
 1002 FORMAT(1I1)                                                       A2   587
 2001 FORMAT(1H016X,11HANGLE INPUT/1H010X,5HTHETA,8X,3HCHI,8X,3HPHI//)  A2   588
 2002 FORMAT(1H (2(A6,3F11.3,6X)))                                      A2   589
      RETURN                                                            A2   590
      END (0,1,0,0,0)                                                   A2   591


C       SUBROUTINE FACE(IDENT,N,DATA,NCOF,DATE), 3 DIMENSIONAL PROBLEM  F1   592
C        BEFORE ENTRY, IDENT, NCOF ARE SET                              F1   593
C        UPON EXIT, SUBROUTINE SUPPLIES N AND COEFFICIENTS WHICH        F1   594
C                   DESCRIBE PLANES FORMING FACES OF CRYSTAL            F1   595
C        NOTATION   IDENT = IDENTIFICATION OF CRYSTAL                   F1   596
C                       N = NUMBER OF FACES                             F1   597
C                    DATA = BLOCK OF GENERAL STORAGE                    F1   598
C                    NCOF = ELEMENT OF DATA CONTAINING FIRST            F1   599
C                           COEFFICIENT DESCRIBING PLANES,  OR FIRST    F1   600
C                           AVAILABLE CELL OF STORAGE UPON ENTRY        F1   601
C                     NOP = 0  IMPLIES DO NOT REPORT INPUT              F1   602
C                         = 1  IMPLIES REPORT INPUT                     F1   603
C                    DATE = BCD DATE                                    F1   604
      SUBROUTINEFACE(IDENT,N,DATA,NCOF,DATE)                            F1   605
      DIMENSION IDENT(12),DATA(1)                                       F1   606
      READINPUTTAPE10,1001,N,NOP                                        F1   607
      NEND=4*N+NCOF-1                                                   F1   608
      READINPUTTAPE10,1002,(DATA(I1),I1=NCOF,NEND)                      F1   609
      IF(NOP)2,2,3                                                      F1   610
    3 NBEG=NCOF                                                         F1   611
      K3=0                                                              F1   612
    7 CALLIDOUT(IDENT,DATE,9)                                           F1   613
      WRITEOUTPUTTAPE9,2001,N                                           F1   614
      DO4K1=NBEG,NEND,4                                                 F1   615
      K2=K1+3                                                           F1   616
```

```
      K3=K3+1                                                           F1   617
      WRITEOUTPUTTAPE9,2002,K3,(DATA(I1),I1=K1,K2)                      F1   618
      IF(50-K3)5,5,4                                                    F1   619
    5 NBEG=K1                                                           F1   620
      GOTO7                                                             F1   621
    4 CONTINUE                                                          F1   622
 1001 FORMAT(2I5)                                                       F1   623
 1002 FORMAT(4E10.8)                                                    F1   624
 2001 FORMAT(1H+,70X,17HNUMBER OF FACES =I5/75HOCOEFFICIENTS A, B, C, D F1   625
     1WHERE  AX + BY + CZ = D  DESCRIBES FACE OF CRYSTAL/1HO,2X,1HN,7X,1F1   626
     2HA,9X,1HB,9X,1HC,9X,1HD//)                                        F1   627
 2002 FORMAT(1H I3,2X,4F10.5)                                           F1   628
    2 RETURN                                                            F1   629
      END(0,1,0,0,0)                                                    F1   630


*       SUBROUTINE SIZE                                                  S   631
      REM TO DETERMINE AMOUNT OF STORAGE AVAILABLE FOR DATA              S   632
      REM MAKE DECREMENT OF SIZE + 5 =PART OF UPPER CORE NOT AVAILABLE   S   633
      REM ENTER WITH  TSX SIZE,4                                         S   634
      REM             HTR NS                                             S   635
      REM EXIT WITH   TRA 2,4                                            S   636
      REM NS WILL CONTAIN AMOUNT OF AVAILABLE STORAGE IN DECREMENT.      S   637
      REM THIS SUBROUTINE MUST BE THE LAST SUBROUTINE LOADED.            S   638
      FUL                                                                S   639
      ORG 0                 PROGRAM CARD                                 S   640
      MZE 0,0,4             9L                                           S   641
      PZE 0                 9R                                           S   642
      PZE END+1             8L                                           S   643
      PZE 0                 8R                                           S   644
      BCD 1SIZE             7L                                           S   645
      PZE 0                 7R                                           S   646
      ORG 0                                                              S   647
      REL                                                                S   648
SIZE  SXD END,4                                                          S   649
      CLA 1,4                                                            S   650
      STA SIZE+6                                                         S   651
      LXA END,4                                                          S   652
      TIX *+1,4,END                                                      S   653
      TIX *+1,4,205                                                      S   654
      SXD 0,4               NS                                           S   655
      LXD END,4                                                          S   656
      TRA 2,4                                                            S   657
END   HTR -1                                                             S   658
      END 0                                                              S   659
```

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```
    8                                                                  M     660
.019855072.101666761.237233795.408282679                               U1    661
.591717321.762766205.898333239.980144928                               U2    662
.050614268.111190517.156853323.181341892                                R1   663
.181341892.156853323.111190517.050614268                               R2    664
```

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OR GLS,

A GENERAL FORTRAN LEAST SQUARES PROGRAM

William R. Busing
Henri A. Levy

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A GENERAL FORTRAN LEAST SQUARES PROGRAM

by

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Chemistry Division

June, 1962

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ABSTRACT

This report describes a computer program which will adjust the parameters of an arbitrary function to fit a set of observed values by the method of least squares. The form of this function is to be defined in terms of a subroutine prepared by the user. The derivatives needed for the method of least squares are either obtained numerically by the program or calculated analytically by the user's subroutine. Most of the program is written in the Fortran language to facilitate any desired modifications and to permit its use on various machines. Instructions are included for the use of the program, which is available in card form from the authors.

INTRODUCTION

The computer program to be described will adjust the parameters of an arbitrary function to obtain a least-squares fit to a set of observations. The function involved may have any form which can be defined by a subprogram, prepared by the user, to obtain its value for a given set of trial parameters and independent variables. The derivatives needed for the method of least squares are either obtained numerically by the program or calculated analytically by the user's subroutine.

The input data to each job include a set of observations, each with its corresponding independent variables, and, if desired, its estimated standard error. The latter determines the weight of the observation unless the use of unit weights is specified. The program also reads a set of trial parameters and an indication of which of these are to be adjusted. If numerical differentiation is to be performed, a parameter increment to be used in this process is associated with each parameter to be varied.

More than one cycle of refinement will be required to converge on the final solution unless the function to be fitted happens to be linear in the variable parameters. The program allows the user to specify the number of cycles to be performed in each job and also permits him to provide a test to terminate the calculation after fewer cycles if appropriate. Provision is made to transfer the parameters from one job to another by means of either magnetic tape or punched cards.

A list comparing the observed and calculated function is put out together with an over-all agreement factor before each cycle of refinement and once more after the last adjustment. The old and new parameters with their calculated standard errors are listed after each cycle, and the correlation matrix is put out at the end of each job.

The program has been used successfully for crystal structure refinements involving more than ninety variables and over two thousand observations. Most of it is written in Fortran to facilitate any desired modifications and to permit its use on various machines. Both symbolic and column binary cards are available from the authors.

GENERAL DESCRIPTION

It is expected that the Fortran listing and the glossary of symbols which are provided will serve as a complete description of the program. The form of the input is described in detail in a separate section, and an example of such input, together with the corresponding output, is also given. This section is therefore intended to serve only as a brief summary of the method.

Of fundamental importance is the user's subroutine CALC which, during each cycle, is entered once for each observation to obtain YC, the value of the function based on the current parameters and the NX independent variables associated with the observation. For each observation the program stores in the array DV the derivatives of YC with respect to those parameters P which are to be varied. If the user elects to have these derivatives obtained numerically, he must associate with each P(I) a parameter increment DP(I). For each of the NV variables the program adds DP(I) to P(I) and re-enters CALC to obtain YD, the function based on the parameters with one incremented. The required derivative is then taken as DV(I) = (YD-YC)/DP(I).

Alternatively, the user may elect to include the analytical calculation of the derivatives in subroutine CALC, and this will save appreciable machine time in problems with complicated functions and many variables. In this case the subroutine is entered only once for each observation, and the derivatives with respect to every possible variable are stored in the array DC at the same time that YC is calculated. The program later selects from this array the derivatives with respect to those parameters to be varied in a particular job.

It is possible to use a combination of numerical and programmed derivatives by specifying numerical derivatives but setting to zero the parameter increments associated with some variables. When the program finds such a zero increment, it assumes that a programmed derivative is to be used for that variable.

Additional flexibility is provided by an optional user's subroutine PRELIM which is entered once at the beginning of each job. This may be used to read various constants, make preliminary computations, and otherwise prepare for the function calculation. It may also be used for data

processing, weight calculation, or other modification of the observation input.

For each cycle the matrix and vector of the normal equations are stored by computing the contributions of one observation at a time. The calculated function and the required derivatives are obtained as described above, and a line of output comparing the observation with its calculated value is put out. The term (SQRTW*DV(J))*(SQRTW*DV(K)) is then added to AM(JK), the J,Kth element of the matrix, where SQRTW is the square root of the weight of the observation. The contribution to the vector element V(J) is (SQRTW*DV(J))*(SQRTW*(YO-YC)), and that to the agreement factor SIG is (SQRTW*(YO-YC))**2. Here YO is used as an abbreviation for YO(I), the Ith observed value of the function.

This process is repeated until the contributions from all the observations have been obtained. At this point an agreement factor, the standard error of an observation of unit weight, SQRTF(SIG/(NO-NV)), is computed and put out.

The storage scheme used for the matrix AM is described in the glossary. To make efficient use of memory space, only the upper triangular part of this symmetric matrix is stored. Furthermore, to conform to the requirements of the existing matrix inverter, SMI, the matrix is stored forward in core or backward in the normal Fortran indexing system.

Before the matrix is inverted it is tested for zero diagonal elements which would indicate a singular matrix with one or more zero row-columns. This would be the result if the derivatives with respect to the corresponding parameters were zero for all observations. A singular matrix due to the attempt to vary sets of parameters with one or more redundancies will be found in the course of the inversion. In case of either type of singularity, the job is terminated with the appropriate comment.

The matrix inversion procedure is described in detail elsewhere (W. R. Busing and H. A. Levy, Comm. ACM, 1962. To be published.) It involves the diagonalization of the matrix by a series of congruent transformations, inversion by taking reciprocals of the diagonal elements, and a sequence of reverse transformations. Upon completion of the process the inverse matrix has replaced the original one in the array AM.

The vector is then multiplied by the inverse matrix to obtain the parameter changes, PD. An estimated new value of the agreement factor SIG is obtained by subtracting from it PD(I)*V(I) summed over the NV variables, and a revised SQRTF(SIG/(NO-NV)) is computed. The entire list of parameters is then put out showing the changes which were made and the estimated standard errors associated with these variables. The latter are computed as SQRTF(DIAG(J)*SIG/(NO-NV)) where DIAG is an array of the diagonal elements of the inverse matrix. It should be noted that these estimates are exact only if the function is linear in the parameters, are approximately correct for converging nonlinear functions, but may be grossly incorrect if the calculation is diverging.

At this point the program enters a subroutine TEST which may be provided at the option of the user. This routine may be used to determine whether the new parameter values are reasonable, modify them if necessary, or terminate the job. It may also be used to test the agreement factors from several cycles so that the job may be terminated when convergence is achieved. Unless the job is ended by TEST or because of a singular matrix, the above procedure will be repeated for the specified number of cycles, and then a final calculation and output of YC will be made.

At the end of the job, unless a singular matrix has been found, the program computes the correlation matrix by dividing each inverse matrix element AM(IJ) by SQRTF(DIAG(I)*DIAG(J)). Only the upper triangular part of this symmetric matrix is reported, and the other elements appear as zero in the listing.

DATA INPUT

*The limitations marked with an asterisk depend only on the dimensions with which the program is compiled.

1. Title card. FORMAT (12A6)

Columns	
1-72	TITLE consisting of any desired Hollerith information. This will be put out as a heading on each section of output.

2. Control card. FORMAT (7I3)

Columns	
1-3	NC, the number of cycles to be run on this job. Calculated values of YC will be listed NC + 1 times. If NC = 0 one list of calculated YC will be put out, but no refinement will be made.

4-6	NV, the number of parameters to be varied. If NC = 0 then NV is irrelevant. $1 \leqslant NV \leqslant 100$.*
7-9	NX, the number of independent variables associated with each observation. $1 \leqslant NX \leqslant 5$.*
10-12	ID, the derivative indicator. ID = 0 indicates that the required derivatives have been programmed by the user. ID = 1 indicates that the required derivatives will be calculated numerically except for parameters which have DP(I) = 0.
13-15	IW, the weight indicator. IW = 0 indicates that individual standard errors will be supplied by the user for each observation. IW = 1 indicates that the program is to weight each observation at unity.
16-18	IP, the parameter input indicator. IP = 0 indicates that trial parameters are supplied as input data. IP > 0 indicates that the program is to read the input parameters from a private tape using those from cycle IP of a previous job.
19-21	IT, the auxiliary output indicator. If IT = 0 the corrected parameters are not to be saved for later use. If IT = 1 the corrected parameters are to be written on a private tape. If IT = 2 the corrected parameters are to be written on an auxiliary output tape to be punched on cards off-line.

3. Trial parameter cards. FORMAT (I3/(8F9.4))
These are to be provided only when IP = 0 on the control card.

First card.
Columns

1-3	NP, the total number of parameters to be read (including those to be varied and those to be held constant). $1 \leqslant NP \leqslant 200$.*

Second card.
Columns

1-9	P(1), the trial value of the first parameter, etc.
10-18	P(2)
19-27	P(3)
.	.
.	.
64-72	P(8)

Third card.

Columns	
1-9	P(9)
10-18	P(10)
.	.
.	.
	P(NP)

4. Observation cards. FORMAT (I1,E8.4,7E9.4/(8E9.4))
Include one or more cards for each of NO observations. $1 \leqslant NO \leqslant 999$.*

Columns	
1	Blank
2-9	YO, the observed value of the dependent variable.
10-18	SIGYO, the standard error of this observation. If IW = 1 on the control card this field is irrelevant.
19-27	X(1), the first independent variable.
28-36	X(2), the second independent variable.
.	.
.	.
.	X(NX), the last independent variable. Note that these fields can be used to input any numbers which pertain to an individual observation. (If it is desired to make NX > 5 then the program must be recompiled with altered dimension statements. If NX = 6 then a second card which is blank must be supplied for each observation unless the FORMAT statement is changed.)

5. Observation termination card. FORMAT (I1)

Column	
1	ISENT = 1 as sentinel for end of observation deck. (If NX $\geqslant$ 6 then blank cards must be added so that the termination includes as many cards as an observation.)

6. Key integer cards. FORMAT (72I1)
These are omitted if NC = 0. Otherwise one card is included for each 72 trial parameters (or fraction thereof) read.

First card.

Column	
1	KI(1) = 0 if P(1) is not to be varied. KI(1) = 1 if P(1) is to be varied.

2	KI(2) associated in the same way with P(2), etc.
.	.
.	.
72	KI(72)

Second card.
Column

1	KI(73)
.	.
.	.
	KI(NP)

7. Parameter increment cards. FORMAT (8E9.4)
These cards are included only if both NC $\geqslant$ 1 and ID = 1, that is, if some of the least squares derivatives are to be computed numerically.

First cards.
Columns

1-9	DP(1), the parameter increment associated with P(1). If the derivative of YC with respect to P(1) is to be determined numerically, DP(1) is the parameter increment which will be added to P(1). If KI(I) = 0 then DP(I) is irrelevant. If KI(I) = 1 and DP(I) = 0 then the program will expect the derivative with respect to P(I) to be calculated by the user's subprogram, CALC.
10-18	DP(2), the parameter increment associated with P(2), etc.
.	.
.	.
64-72	DP(8)

Second card.
Columns

1-9	DP(9)
.	.
.	.
	DP(NP)

8. Any data to be read by the user's subroutine PRELIM.

TAPES REQUIRED

Listed here are the monitor tape control cards required for operation at the Oak Ridge Central Data Processing Facility. At other installations the necessary tapes should be specified appropriately.

*TAPE(4, Reel number, SAVE)

This is required only if IP > 0 indicating that the initial values of the trial parameters are to be taken from this tape, which was written on a previous job.

*TAPE(5, POOL, SAVE)

This is required only if IT = 1 indicating that the adjusted parameters are to be written on this tape after each cycle. This tape is initially rewound and an end-of-file is written upon completion of the job.

*TAPE(6, AUXOUT)

This is required only if IT = 2 indicating that the adjusted parameters are to be written on this tape after each cycle. Cards suitable for input to another job will then be punched off-line. This tape is not rewound and no end-of-file is written on it by the program.

*TAPE(9, OUTPUT)

*TAPE(10, INPUT)

SUBROUTINES TO BE SUPPLIED BY THE USER

SUBROUTINE CALC(XI,Y,P,D)

This subroutine must be supplied by the user to evaluate the function and to calculate the necessary derivatives if these are to be programmed.

The argument XI is used as a vector of the NX independent variables for one observation. This vector represents column I of the two dimensional calling program array X, and the CALL statement for observation I uses the argument X(1,I). If NX > 1 then XI must be included in a DIMENSION statement. Note that this array may be used to convey to the subroutine any information which pertains to a particular observation.

Y is the single valued function to be calculated. The calling program uses either YC or YD as the corresponding argument.

P is the array of trial parameters some of which are to be varied. It should be included in a DIMENSION statement. This array may also be used to convey constants or instructions to the subroutine, but such parameters should not be adjusted.

D is the array in which derivatives are to be stored if they are calculated by this subroutine. It is in one to one correspondence with

the array P. The calling program refers to it as DC or DD. The array should be included in a DIMENSION statement.

If COMMON storage is used for communication with subroutine PRELIM (see below) then care should be taken to include the COMMON and DIMENSION statements from the calling program.

The user must program the calculation of Y from the independent variables XI and the parameters P. If derivatives are programmed, then $\partial Y/\partial P(J)$ should be stored in D(J), etc. Only derivatives with respect to parameters to be varied need be programmed, but storing derivatives which will not be used is permitted. Programming the derivative calculation will save appreciable machine time on problems with complicated functions and many variables. The derivative programming can often be checked by comparing the results of a least-squares cycle which uses it with those of the same cycle using numerical differentiation.

The usual RETURN and END statements are added, and the compiled program is inserted before the transfer card in the program deck.

SUBROUTINE PRELIM

This optional subroutine is entered once after all the input has been read but before the initial values of the trial parameters are put out. It may be used to read additional input, make preliminary calculations, and otherwise prepare subroutine CALC for the function computation. In its present form the main program provides no arguments for PRELIM, and it is expected that COMMON storage will be used to communicate with CALC.

The subroutine must include COMMON and DIMENSION statements exactly as they appear in the main program, preceding any COMMON statements inserted by the user.

The usual RETURN and END statements are added, and the compiled program is substituted for the dummy program which is included with the card deck provided.

SUBROUTINE TEST

This optional subroutine is entered once at the end of each cycle after the parameters have been adjusted and listed but before they are put out on tape or cards for use in another job. It may be used to test

whether the new parameter values are reasonable, modify them if desired, or terminate the job. It may also be used to test for convergence of the least-squares procedure.

No arguments are provided by the calling program in its present form, but communication may be made by means of COMMON storage.

The subroutine must include COMMON and DIMENSION statements exactly as they appear in the main program, preceding any COMMON statements inserted by the user.

Before TEST is called, the main program sets ISTOP to zero. If the job is to be terminated, TEST should set ISTOP to a non-zero integer. When a job is terminated in this way, the value of ISTOP is given in the output listing so that it may be used as an indicator to identify one of several reasons for stopping.

The array SQSIG may be used as the basis of a test for convergence. When TEST is called, SQSIG(1) contains the estimated agreement factor SQRTF(SIG/(NO-NV)) for the new parameters. For comparison SQSIG(2) contains the same quantity from the previous cycle. On the first cycle of each job SQSIG(2) is zero.

The usual RETURN and END statements are added, and the compiled program is substituted for the dummy routine which is included in the card deck provided.

CARD DECKS PROVIDED

Subprogram	Type	Symbolic card numbers	Column binary card numbers*
Calling program	Fortran	1 - 384	691 - 756
PRELIM (dummy)	Fortran	385 - 389	757 - 758
TEST (dummy)	Fortran	390 - 394	759 - 760
SMI	FAP	395 - 647	761 - 774
CALC (example)	Fortran	648 - 666	775 - 779

Library subroutines to be inserted here if not supplied by monitor system.

Transfer card	667
Data for example	668 - 690

*These column binary cards were compiled or assembled on an IBM 7090. For use on a 704 the calling program should be recompiled, but the remaining subprograms which are included here should be satisfactory.

LIBRARY SUBROUTINES

At the Oak Ridge Central Data Processing Facility all necessary subroutines, except those described above, are supplied from the monitor library tape. At other installations the following subroutines should be provided: Fortran input-output routines, SQRT, FPTRP, ERROR, and EXIT.

FPTRP initializes a floating trap routine so that underflows are set to zero and overflows cause a transfer to ERROR. ERROR terminates the calculation and initiates an optional memory dump. A job is normally ended by calling EXIT.

GLOSSARY OF SYMBOLS

*Indicates input data.

A. Single Storage Variables

* NC	Number of cycles of refinement to be performed in this job. The program puts out YC, the values of the calculated function, NC + 1 times. If NC = 0, YC is calculated, but no refinement occurs.
* NV	Number of parameters to be varied. If NC = 0 then NV is irrelevant.
* NX	Number of independent variables associated with each observation.
* ID	Derivative calculation indicator. If ID = 0 it is assumed that the user's subroutine CALC calculates the derivatives and stores them in DC. If ID = 1 derivatives are to be calculated numerically (except for those parameters for which DP(I) = 0).
* IW	Unit weight indicator. If IW = 1 all observations are assigned unit weights. If IW = 0 then the weights are taken as 1.0/SIGYO(I)**2.
* IP	Parameter input indicator. If IP = 0 the parameters P are to be read from cards. If IP > 0 then the parameters are to be taken from the magnetic tape output of cycle IP of a previous job.
* IT	Parameter output indicator. If IT = 0 parameters are not to be written on tape for later use, if IT = 1 they are to be written on a private tape, and it IT = 2 they are written on the monitor auxiliary tape in such a way as to yield punched

	cards. The private tape is initially rewound and is terminated by an end-of-file while the auxiliary tape is not.
* NP	Total number of parameters including those to be varied as well as those to be held constant.
NO	Number of observations.
IC	Identifying number of a particular cycle in this job.
NCY	NC + 1, the number of cycles plus one. This is the number of times the list of YC will be put out.
SIG	(SQRTW*(YO-YC))**2 summed over all observations.
SQRTW	Square root of the weight for each observation.
YC	Calculated value of the function stored by subroutine CALC.
YD	Calculated value of the function as stored by subroutine CALC for computing numerical derivatives.
DY	YO-YC
WDY	(YO-YC)/SIGYO(I)
PSAVE	Parameter saved while original is incremented for numerical differentiation.
NM	(NV*(NV + 1))/2, the number of elements in the matrix.
SIGP	Standard error of a parameter.
ISTOP	Stop indicator set $\neq$ 0 by subroutine TEST to indicate that no further cycles are to be run on this job. Otherwise ISTOP = 0.
* ISENT	Sentinel set at 1 to end observation deck.
DPK	DP(K) saved for derivative calculation.
PDI	PD(I)
JK	Index used so that AM(JK) is a_{jk}.
IJ	Index used so that AM(IJ) is a_{ij}.
IJD	Increment subtracted from IJ to step down a column of matrix AM(IJ).

POLD	Parameter before correction is added. Saved for output.
II	Index used so that AM(II) is diagonal element a_{ii}.
IID	Increment subtracted from II to step down diagonal of matrix AM(II).
ISING	Singularity indicator set at 1 if a zero diagonal element is found in the original matrix or if a diagonal element becomes zero or negative during inversion by SMI. Otherwise ISING = 0.
NPCD	Multiple of 8 greater than or equal to NP.
NT	Number of private or auxiliary tape used for output of parameters to be saved.

B. Arrays With Their Minimum Dimensions.

* TITLE(12)	Alphanumeric title read at start of problem and transcribed to the output.
* P(NP)	List of NP parameters, some of which will be varied.
* DP(NP)	List of increments to be used if numerical differentation is to be performed.
* KI(NP)	Key integers corresponding to the parameters. KI(I) = 1 if P(I) is to be varied. Otherwise KI(I) = 0.
* X(NX,NO)	NX independent variables for each of NO observations.
* YO(NO)	NO observed dependent variables.
* SIGYO(NO)	Standard errors of the NO observations.
AM((NV*(NV+3))/2)	Matrix of the normal equations. This area is also used for the inverse matrix. Only (NV*(NV+1))/2 words are used for the matrix, but NV more are used by the inverter. Only the upper right triangle of the matrix is stored, and this is stored forward in the memory - i.e., backward in the Fortran indexing system. If a_{ij} represents a matrix element than a_{11} is at AM((NV*(NV+1))/2), a_{12} at AM((NV*(NV+1))/2 - 1), etc., a_{22} is at AM((NV*(NV+1))/2 - NV), and $a_{NV,NV}$ is at AM(1). For example if NV = 4 the storage is as illustrated:

a_{11} = AM(10)	a_{12} = AM(9)	a_{13} = AM(8)	a_{14} = AM(7)
	a_{22} = AM(6)	a_{23} = AM(5)	a_{24} = AM(4)
		a_{33} = AM(3)	a_{34} AM(2)
			a_{44} = AM(1)

V(NV)	Vector of the normal equations.
DC(NP)	Calculated derivatives of YC with respect to P. If derivatives are programmed they are stored here by the user's subroutine.
DV(NV)	Derivatives of those parameters which are to be varied multiplied by the square root of the weight.
PD(NV)	Calculated parameter changes for those parameters which were varied.
DIAG(NV)	Diagonal elements of the inverse matrix. These are used for calculating the standard errors of the parameters which were varied.
DD(NP)	Irrelevant derivatives calculated by CALC on entry for numerical derivatives. This array is needed because both numerical and calculated derivatives may be used in the same problem.
SQSIG(2)	SQSIG(1) is the error of fit, SQRTF(SIG/FLOATF(NO-NV)). SQSIG(2) is SQSIG(1) saved from the previous cycle of this job. SQSIG(2) will be set to zero for the first cycle of each job.
ROW(NV)	A row of the correlation matrix ready for output.

```
*TYPE(FORTRAN)                                                          ORGLS  1
C     OR GLS, GENERAL FORTRAN LEAST SQUARES                             ORGLS  2
      COMMON NC,NV,NX,ID,IW,IP,IT,NP,ISENT,NO,NM,NCY,IC,SIG,YC          ORGLS  3
      COMMON SQRTW,DY,WDY,DPK,PSAVE,YD,JK,ISING,II,IID,PDI,IJ,IJD,POLD  ORGLS  4
      COMMON SIGP,ISTOP,NT,NPCD                                         ORGLS  5
      COMMON TITLE,P,X,YO,SIGYO,KI,DP,SQSIG,AM,V,DC,DV,DD,DIAG,PD,ROW   ORGLS  6
                                                                        ORGLS  7
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#200,NO(MAX)#1000,NX(MAX)#5     ORGLS  8
      DIMENSION TITLE(12),P(200),X(5,1000),YO(1000),SIGYO(1000),KI(200) ORGLS  9
      DIMENSION DP(200),SQSIG(2),AM(5150),V(100),DC(200),DV(100),DD(200)ORGLS 10
      DIMENSION DIAG(100),PD(100),ROW(100)                              ORGLS 11
                                                                        ORGLS 12
C     FORMAT STATEMENTS                                                 ORGLS 13
00051 FORMAT(12A6)                                                      ORGLS 14
00052 FORMAT(1H112A6)                                                   ORGLS 15
00053 FORMAT(24I3)                                                      ORGLS 16
00054 FORMAT(32H0NUMBER OF CYCLES IN THIS JOB ISI2/37H0NUMBER OF PARAMETORGLS 17
     1ERS TO BE VARIED ISI3/51H0NUMBER OF INDEPENDENT VARIABLES PER OBSEORGLS 18
     2RVATION ISI2)                                                     ORGLS 19
00058 FORMAT(31H0DERIVATIVES PROGRAMMED BY USER)                        ORGLS 20
00059 FORMAT(57H0NUMERICAL DERIVATIVES UNLESS PARAMETER INCREMENT IS ZERORGLS 21
     10)                                                                ORGLS 22
00061 FORMAT(31H0WEIGHTS TO BE SUPPLIED BY USER)                        ORGLS 23
00062 FORMAT(34H0UNIT WEIGHTS TO BE SET BY PROGRAM)                     ORGLS 24
00063 FORMAT(36H0PARAMETERS TO BE READ AS INPUT DATA)                   ORGLS 25
00064 FORMAT(34H0PARAMETERS TO BE TAKEN FROM CYCLEI2,16H OF PREVIOUS JOBORGLS 26
     1)                                                                 ORGLS 27
00066 FORMAT(I3,81X/(8F9.4,12X))                                        ORGLS 28
00067 FORMAT(29H0NUMBER OF PARAMETERS READ ISI3)                        ORGLS 29
00068 FORMAT(I1,E8.4,7E9.4/(8E9.4))                                     ORGLS 30
00069 FORMAT(31H0NUMBER OF OBSERVATIONS READ ISI4)                      ORGLS 31
00070 FORMAT(72I1)                                                      ORGLS 32
00071 FORMAT(8E9.4)                                                     ORGLS 33
00072 FORMAT(46H0CALCULATED Y BASED ON PARAMETERS BEFORE CYCLEI2)       ORGLS 34
00073 FORMAT(59H0   Y(OBS)   Y(CALC)   OBS-CALC   SIG(O) (O-C)/SIG(O)  XORGLS 35
     1(I)/1H )                                                          ORGLS 36
00079 FORMAT(1H 11F10.4)                                                ORGLS 37
00080 FORMAT(51H0AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE I2/ ORGLS 38
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```
     120HOSUM(W*(O-C)**2) IS E11.4/35HOSQRTF(SUM(W*(O-C)**2)/(NO-NV)) ISORGLS 39
     2 F10.4)                                                         ORGLS 40
00081 FORMAT(60HOESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CORGLS 41
     1YCLE I2/20HOSUM(W*(O-C)**2) IS E11.4/35HOSQRTF(SUM(W*(O-C)**2)/(NOORGLS 42
     2-NV)) IS F10.4)                                                 ORGLS 43
00083 FORMAT(62H MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PARORGLS 44
     1AMETERI3,16H OF THOSE VARIED)                                   ORGLS 45
00085 FORMAT(40H SINGULARITY RETURN FROM MATRIX INVERTER)             ORGLS 46
00086 FORMAT(37HOPARAMETERS AFTER LEAST SQUARES CYCLEI2/43HO        OLD ORGLS 47
     1    CHANGE      NEW       ERROR/1H )                            ORGLS 48
00088 FORMAT(1H I3,F10.4,10X,F10.4)                                   ORGLS 49
00089 FORMAT(1H I3,4F10.4)                                            ORGLS 50
00090 FORMAT(66HOSUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED ORGLS 51
     1FOR REASONI2)                                                   ORGLS 52
00092 FORMAT(11HOINPUT DATA/30HO  I     P(I)  KI(I)     DP(I)/1H )    ORGLS 53
00093 FORMAT(1H I3,F10.4,I4,3X,E11.4)                                 ORGLS 54
00094 FORMAT(51HOCORRECTED PARAMETERS NOT TO BE SAVED FOR LATER USE)  ORGLS 55
00095 FORMAT(51HOCORRECTED PARAMETERS TO BE WRITTEN ON PRIVATE TAPE)  ORGLS 56
00096 FORMAT(51HOCORRECTED PARAMETERS TO BE WRITTEN FOR CARD OUTPUT)  ORGLS 57
00097 FORMAT(19HOCORRELATION MATRIX)                                  ORGLS 58
00098 FORMAT(1HOI3,10F9.4/(1H 3X,10F9.4))                             ORGLS 59
                                                                      ORGLS 60
C     READ TITLE AND CONTROL CARD                                     ORGLS 61
      READ INPUT TAPE 10,00051,(TITLE(I),I#1,12)                      ORGLS 62
      WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                     ORGLS 63
      DUMMY#FPTRPF( 0,-1)                                             ORGLS 64
      READ INPUT TAPE 10,00053,NC,NV,NX,ID,IW,IP,IT                   ORGLS 65
      WRITE OUTPUT TAPE 9,00054,NC,NV,NX                              ORGLS 66
      IF(ID)00206,00204,00206                                         ORGLS 67
                                                                      ORGLS 68
00204    WRITE OUTPUT TAPE 9,00058                                    ORGLS 69
         GO TO 00207                                                  ORGLS 70
                                                                      ORGLS 71
00206    WRITE OUTPUT TAPE 9,00059                                    ORGLS 72
                                                                      ORGLS 73
00207 IF(IW)00210,00208,00210                                         ORGLS 74
                                                                      ORGLS 75
00208    WRITE OUTPUT TAPE 9,00061                                    ORGLS 76
```

```
      GO TO 00211                                                       ORGLS 77
                                                                        ORGLS 78
00210 WRITE OUTPUT TAPE 9,00062                                         ORGLS 79
                                                                        ORGLS 80
00211 IF(IP)00212,00212,00214                                           ORGLS 81
                                                                        ORGLS 82
00212 WRITE OUTPUT TAPE 9,00063                                         ORGLS 83
      GO TO 00215                                                       ORGLS 84
                                                                        ORGLS 85
00214 WRITE OUTPUT TAPE 9,00064,IP                                      ORGLS 86
                                                                        ORGLS 87
00215 IF(IT-1)00216,00218,00221                                         ORGLS 88
                                                                        ORGLS 89
00216 WRITE OUTPUT TAPE 9,00094                                         ORGLS 90
      GO TO 00301                                                       ORGLS 91
                                                                        ORGLS 92
00218 WRITE OUTPUT TAPE 9,00095                                         ORGLS 93
      REWIND 5                                                          ORGLS 94
      GO TO 00301                                                       ORGLS 95
                                                                        ORGLS 96
00221 WRITE OUTPUT TAPE 9,00096                                         ORGLS 97
                                                                        ORGLS 98
C     READ TRIAL PARAMETERS                                             ORGLS 99
00301 IF(IP)00401,00401,00501                                           ORGLS100
                                                                        ORGLS101
00401 READ INPUT TAPE 10,00066,NP,(P(I),I#1,NP)                         ORGLS102
      GO TO 00601                                                       ORGLS103
                                                                        ORGLS104
00501 REWIND 4                                                          ORGLS105
      DO 00503 J#1,IP                                                   ORGLS106
                                                                        ORGLS107
00503    READ INPUT TAPE 4,00066,NP,(P(I),I#1,NP)                       ORGLS108
                                                                        ORGLS109
00601 WRITE OUTPUT TAPE 9,00067,NP                                      ORGLS110
                                                                        ORGLS111
C     READ OBSERVATIONS TO SENTINEL                                     ORGLS112
      J#0                                                               ORGLS113
                                                                        ORGLS114
```

```
00801     J#J+1                                                          ORGLS115
          READ INPUT TAPE IO,00068,ISENT,YO(J),SIGYO(J),(X(I,J),I#1,NX)  ORGLS116
          IF(ISENT)00801,00801,01101                                     ORGLS117
                                                                         ORGLS118
01101 NO#J-1                                                             ORGLS119
      WRITE OUTPUT TAPE 9,00069,NO                                       ORGLS120
                                                                         ORGLS121
C     READ KEY INTEGERS AND PARAMETER INCREMENTS IF SPECIFIED            ORGLS122
      IF(NC)01601,01601,01301                                            ORGLS123
                                                                         ORGLS124
01301     READ INPUT TAPE IO,00070,(KI(I),I#1,NP)                        ORGLS125
          IF(ID)01501,01601,01501                                        ORGLS126
                                                                         ORGLS127
01501         READ INPUT TAPE IO,00071,(DP(I),I#1,NP)                    ORGLS128
                                                                         ORGLS129
C     INITIALIZE PROBLEM AND ENTER SUBROUTINE PRELIM IF PROVIDED         ORGLS130
01601 NM#(NV*(NV+1))/2                                                   ORGLS131
      SQSIG(1)#0.0                                                       ORGLS132
      CALL PRELIM                                                        ORGLS133
                                                                         ORGLS134
C     PUT OUT TRIAL PARAMETERS, KEY INTEGERS, AND PARAMETER INCREMENTS   ORGLS135
      WRITE OUTPUT TAPE 9,00092                                          ORGLS136
      DO 01653 I#1,NP                                                    ORGLS137
                                                                         ORGLS138
01653     WRITE OUTPUT TAPE 9,00093,I,P(I),KI(I),DP(I)                   ORGLS139
                                                                         ORGLS140
C     START LOOP TO PERFORM NC CYCLES AND ONE FINAL CALCULATION OF Y     ORGLS141
      NCY#NC+1                                                           ORGLS142
      DO 08501 IC#1,NCY                                                  ORGLS143
                                                                         ORGLS144
C         CLEAR ARRAYS AM AND V EXCEPT ON LAST CYCLE                     ORGLS145
          IF(IC-NCY)01851,02001,02001                                    ORGLS146
                                                                         ORGLS147
01851         DO 01852 I#1,NM                                            ORGLS148
                                                                         ORGLS149
01852             AM(I)#0.0                                              ORGLS150
                                                                         ORGLS151
              DO 01902 I#1,NV                                            ORGLS152
```

```
                                                                        ORGLS153
01902          V(I)#0.0                                                 ORGLS154
                                                                        ORGLS155
C        INITIALIZE FOR CYCLE IC AND PUT OUT CAPTION FOR LIST OF Y(CALC)ORGLS156
02001    SQSIG(2)#SQSIG(1)                                              ORGLS157
         SIG#0.0                                                        ORGLS158
         WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                    ORGLS159
         WRITE OUTPUT TAPE 9,00072,IC                                   ORGLS160
         WRITE OUTPUT TAPE 9,00073                                      ORGLS161
                                                                        ORGLS162
C        START LOOP THROUGH NO OBSERVATIONS                             ORGLS163
02201    DO 05101 I#1,NO                                                ORGLS164
                                                                        ORGLS165
C           ENTER USERS SUBROUTINE TO COMPUTE Y(CALC) AND DERIVATIVES   ORGLS166
            CALL CALC(X(1,I),YC,P,DC)                                   ORGLS167
                                                                        ORGLS168
C           OBTAIN WEIGHT AND CALCULATE QUANTITIES FROM Y(OBS)-Y(CALC)  ORGLS169
            IF(IW)02601,02501,02601                                     ORGLS170
                                                                        ORGLS171
02501          SQRTW#1.0/SIGYO(I)                                       ORGLS172
               GO TO 02701                                              ORGLS173
                                                                        ORGLS174
02601          SIGYO(I)#1.0                                             ORGLS175
               SQRTW#1.0                                                ORGLS176
                                                                        ORGLS177
02701       DY#YO(I)-YC                                                 ORGLS178
            WDY#SQRTW*DY                                                ORGLS179
            SIG#SIG+WDY*WDY                                             ORGLS180
                                                                        ORGLS181
C           PUT OUT Y(CALC) AND OTHER INFORMATION FOR ONE OBSERVATION   ORGLS182
            WRITE OUTPUT TAPE 9,00079,YO(I),YC,DY,SIGYO(I),WDY,(X(J,I), ORGLS183
     1                                                     J#1,NX)      ORGLS184
                                                                        ORGLS185
C           BY-PASS DERIVATIVE AND MATRIX SET-UP ON FINAL CALC OF Y     ORGLS186
            IF(IC-NCY)03001,05101,05101                                 ORGLS187
                                                                        ORGLS188
C              START LOOP TO STORE AN ARRAY OF NV DERIVATIVES           ORGLS189
03001          J#1                                                      ORGLS190
```

```
                DO 0401 K#1,NP                                          ORGLS191
                                                                        ORGLS192
                   IF(KI(K))0401,0401,0320I                             ORGLS193
                                                                        ORGLS194
0320I                 IF(ID)0340I,0330I,0340I                           ORGLS195
                                                                        ORGLS196
C                        OBTAIN DERIVATIVE FROM THOSE PROGRAMMED BY USER ORGLS197
0330I                    DV(J)#SQRTW*DC(K)                              ORGLS198
                         GO TO 0400I                                    ORGLS199
                                                                        ORGLS200
C                        OBTAIN DERIVATIVE NUMERICALLY UNLESS PARAMETER ORGLS201
C                                                INCREMENT IS ZERO      ORGLS202
0340I                    DPK#DP(K)                                      ORGLS203
                         IF(DPK)0360I,0330I,0360I                       ORGLS204
                                                                        ORGLS205
0360I                       PSAVE#P(K)                                  ORGLS206
                            P(K)#PSAVE+DPK                              ORGLS207
                            CALL CALC(X(1,I),YD,P,DD)                   ORGLS208
                            DV(J)#SQRTW*(YD-YC)/DPK                     ORGLS209
                            P(K)#PSAVE                                  ORGLS210
                                                                        ORGLS211
0400I              J#J+1                                                ORGLS212
0401I              CONTINUE                                             ORGLS213
C                  END LOOP TO OBTAIN DERIVATIVES                       ORGLS214
                                                                        ORGLS215
C               START LOOP TO STORE MATRIX AND VECTOR. SEE GLOSSARY FOR ORGLS216
C                                                STORAGE SCHEME         ORGLS217
                JK#NM                                                   ORGLS218
                DO 0500I J#1,NV                                         ORGLS219
                                                                        ORGLS220
0430I              IF(DV(J))0450I,0440I,0450I                           ORGLS221
                                                                        ORGLS222
C                     BY-PASS IF DERIVATIVE IS ZERO                     ORGLS223
0440I                 JK#JK-NV+J-1                                      ORGLS224
                      GO TO 0500I                                       ORGLS225
                                                                        ORGLS226
0450I                 DO 0480I K#J,NV                                   ORGLS227
                                                                        ORGLS228
```

```
                    AM(JK)#AM(JK)+DV(J)*DV(K)                          ORGLS229
                    JK#JK-1                                            ORGLS230
04801               CONTINUE                                           ORGLS231
                                                                       ORGLS232
                 V(J)#V(J)+DV(J)*WDY                                   ORGLS233
05001            CONTINUE                                              ORGLS234
C                END LOOP TO STORE MATRIX AND VECTOR                   ORGLS235
                                                                       ORGLS236
05101         CONTINUE                                                 ORGLS237
C             END LOOP THROUGH NO OBSERVATIONS                         ORGLS238
                                                                       ORGLS239
C        COMPUTE AND PUT OUT AGREEMENT FACTORS                         ORGLS240
         SQSIG(I)#SQRTF(SIG/FLOATF(NO-NV))                             ORGLS241
         WRITE OUTPUT TAPE 9,00080,IC,SIG,SQSIG(I)                     ORGLS242
                                                                       ORGLS243
C        BY-PASS MATRIX INVERSION AND PARAMETER OUTPUT ON FINAL CYCLE  ORGLS244
         IF(IC-NCY)05401,08701,08701                                   ORGLS245
                                                                       ORGLS246
C           START LOOP TO TEST FOR ZERO DIAGONAL ELEMENT               ORGLS247
05401       ISING#0                                                    ORGLS248
            II#NM                                                      ORGLS249
            IID#NV                                                     ORGLS250
            DO 05801 I#1,NV                                            ORGLS251
                                                                       ORGLS252
               IF(AM(II))05701,05601,05701                             ORGLS253
                                                                       ORGLS254
05601             ISING#1                                              ORGLS255
                  WRITE OUTPUT TAPE 9,00083,I                          ORGLS256
                                                                       ORGLS257
05701          II#II-IID                                               ORGLS258
               IID#IID-1                                               ORGLS259
05801          CONTINUE                                                ORGLS260
C              END LOOP TO TEST FOR ZERO DIAGONAL ELEMENT              ORGLS261
                                                                       ORGLS262
C           TERMINATE JOB IF ZERO DIAGONAL ELEMENT WAS FOUND           ORGLS263
            IF(ISING)10301,06001,10301                                 ORGLS264
                                                                       ORGLS265
C              ENTER SUBROUTINE TO REPLACE MATRIX WITH INVERSE         ORGLS266
```

```
06001          CALL SMI(AM(NM),NV,ISING)                                ORGLS267
               IF(ISING)06201,06301,06201                               ORGLS268
                                                                        ORGLS269
C                 TERMINATE JOB IF SINGULAR MATRIX WAS FOUND            ORGLS270
06201             WRITE OUTPUT TAPE 9,00085                             ORGLS271
                  GO TO 10301                                           ORGLS272
                                                                        ORGLS273
C                 START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR       ORGLS274
C                                              PARAMETER CHANGES        ORGLS275
06301             DO 07201 I#1,NV                                       ORGLS276
                                                                        ORGLS277
                     PDI#0.0                                            ORGLS278
                     IJ#NM-I+1                                          ORGLS279
                     IJD#NV-1                                           ORGLS280
                     DO 07001 J#1,NV                                    ORGLS281
                                                                        ORGLS282
                        PDI#PDI+AM(IJ)*V(J)                             ORGLS283
                        IF(J-I)06701,06801,06901                        ORGLS284
                                                                        ORGLS285
06701                      IJ#IJ-IJD                                    ORGLS286
                           IJD#IJD-1                                    ORGLS287
                           GO TO 07001                                  ORGLS288
                                                                        ORGLS289
C                          SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX     ORGLS290
06801                      DIAG(I)#AM(IJ)                               ORGLS291
                                                                        ORGLS292
06901                      IJ#IJ-1                                      ORGLS293
07001                      CONTINUE                                     ORGLS294
                                                                        ORGLS295
                     PD(I)#PDI                                          ORGLS296
                     SIG#SIG-PDI*V(I)                                   ORGLS297
07201                CONTINUE                                           ORGLS298
C                    END LOOP FOR MATRIX VECTOR MULTIPLICATION          ORGLS299
                                                                        ORGLS300
C                 RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG         ORGLS301
                  SQSIG(1)#SQRTF(SIG/FLOATF(NO-NV))                     ORGLS302
                                                                        ORGLS303
C                 PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS      ORGLS304
```

```
                WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)          ORGLS305
                WRITE OUTPUT TAPE 9,00086,IC                         ORGLS306
C               START LOOP TO CORRECT AND PUT OUT PARAMETERS         ORGLS307
                                                                     ORGLS308
                J#1                                                  ORGLS309
                DO 08001 I#1,NP                                      ORGLS310
                                                                     ORGLS311
                   IF(KI(I))07601,07601,07701                        ORGLS312
                                                                     ORGLS313
07601                 WRITE OUTPUT TAPE 9,00088,I,P(I),P(I)          ORGLS314
                      GO TO 08001                                    ORGLS315
                                                                     ORGLS316
07701                 POLD#P(I)                                      ORGLS317
                      P(I)#POLD+PD(J)                                ORGLS318
                      SIGP#SQRTF(DIAG(J))*SQSIG(I)                   ORGLS319
                      WRITE OUTPUT TAPE 9,00089,I,POLD,PD(J),P(I),SIGPORGLS320
                      J#J+1                                          ORGLS321
                                                                     ORGLS322
08001              CONTINUE                                          ORGLS323
C                  END LOOP TO CORRECT AND PUT OUT PARAMETERS        ORGLS324
                                                                     ORGLS325
C               PUT OUT ESTIMATED AGREEMENT FACTORS                  ORGLS326
                WRITE OUTPUT TAPE 9,00081,IC,SIG,SQSIG(I)            ORGLS327
                                                                     ORGLS328
C               ENTER USERS SUBROUTINE TO TEST AND MODIFY PARAMETERS ORGLS329
C                                                 OR END JOB         ORGLS330
                ISTOP#0                                              ORGLS331
                CALL TEST                                            ORGLS332
                                                                     ORGLS333
C               WRITE CORRECTED PARAMETERS ON AUXILIARY TAPE IF      ORGLS334
C                                                DESIRED             ORGLS335
08201           IF(IT)08202,08301,08202                              ORGLS336
                                                                     ORGLS337
08202              NT#IT+4                                           ORGLS338
                   NPCD#8*((NP-1)/8+1)                               ORGLS339
                   WRITE OUTPUT TAPE NT,00066,NP,(P(I),I#1,NPCD)     ORGLS340
                                                                     ORGLS341
C               TERMINATE JOB IF INDICATED BY USERS SUBROUTINE TEST  ORGLS342
```

```
08301              IF(ISTOP)08401,08501,08401                                ORGLS343
                                                                             ORGLS344
08401                 WRITE OUTPUT TAPE 9,00090,ISTOP                        ORGLS345
                      GO TO 08701                                            ORGLS346
                                                                             ORGLS347
08501                 CONTINUE                                               ORGLS348
C                     END LOOP THROUGH NC CYCLES AND FINAL CALC OF Y         ORGLS349
                                                                             ORGLS350
C     TERMINATE JOB                                                          ORGLS351
08701 IF(NC)10501,10501,08801                                                ORGLS352
                                                                             ORGLS353
C        CALCULATE AND PUT OUT CORRELATION MATRIX                            ORGLS354
08801    WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                         ORGLS355
         WRITE OUTPUT TAPE 9,00097                                           ORGLS356
         DO 09101 I#1,NV                                                     ORGLS357
                                                                             ORGLS358
            DIAG(I)#1.0/SQRTF(DIAG(I))                                       ORGLS359
09101       CONTINUE                                                         ORGLS360
                                                                             ORGLS361
         IJ#NM                                                               ORGLS362
         DO 10201 I#1,NV                                                     ORGLS363
                                                                             ORGLS364
            DO 09601 J#1,NV                                                  ORGLS365
                                                                             ORGLS366
               ROW(J)#0.0                                                    ORGLS367
09601          CONTINUE                                                      ORGLS368
                                                                             ORGLS369
            DO 10001 J#I,NV                                                  ORGLS370
                                                                             ORGLS371
               ROW(J)#AM(IJ)*DIAG(I)*DIAG(J)                                 ORGLS372
               IJ#IJ-1                                                       ORGLS373
10001          CONTINUE                                                      ORGLS374
                                                                             ORGLS375
            WRITE OUTPUT TAPE 9,00098,I,(ROW(J),J#1,NV)                      ORGLS376
10201       CONTINUE                                                         ORGLS377
                                                                             ORGLS378
10301 IF(IT-1)10501,10401,10501                                              ORGLS379
                                                                             ORGLS380
```

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```
10401     END FILE 5                                                    ORGLS381
                                                                        ORGLS382
10501 CALL EXIT                                                         ORGLS383
      END(0,1,0,0,0)                                                    ORGLS384


*TYPE(FORTRAN)                                                          ORGLS385
C     DUMMY SUBROUTINE PRELIM                                           ORGLS386
      SUBROUTINE PRELIM                                                 ORGLS387
      RETURN                                                            ORGLS388
      END                                                               ORGLS389


*TYPE(FORTRAN)                                                          ORGLS390
C     DUMMY SUBROUTINE TEST                                             ORGLS391
      SUBROUTINE TEST                                                   ORGLS392
      RETURN                                                            ORGLS393
      END                                                               ORGLS394


*TYPE(FAP)                                                              ORGLS395
       COUNT   230                                                      ORGLS396
       REM SYMMETRIC MATRIX INVERSE. SEE GLOSSARY FOR STORAGE SCHEME.   ORGLS397
       REM FOR USE ON 704, 709, OR 7090.                                ORGLS398
       REM WRITTEN IN FAP FOR ASSEMBLY ON 709 OR 7090.                  ORGLS399
       ENTRY   SMI                                                      ORGLS400
 SMI   SXD T13,1                                                        ORGLS401
       SXD T14,2                                                        ORGLS402
       LFTM                                                             ORGLS403
       TNO *+1                        OVERFLOW TOGGLES                  ORGLS404
       CAL 1,4                                                          ORGLS405
       COM                                                              ORGLS406
       PAX 0,2                                                          ORGLS407
       TXI *+1,2,1                                                      ORGLS408
       CLA 2,4                                                          ORGLS409
```

```
        STA Y1                                                  ORGLS410
        CLA 3,4                                                 ORGLS411
        STA Y28                                                 ORGLS412
        STA SINGI                                               ORGLS413
Y1      CLA 0                   ADD SET                         ORGLS414
        PDX 0,1                                                 ORGLS415
        STD Y27                                                 ORGLS416
        SXD T1,4                                                ORGLS417
Y2      SXD Y25,1               Y2                              ORGLS418
        SXD T2,1                                                ORGLS419
        SXD T3,2                                                ORGLS420
        STZ T4                  Y3                              ORGLS421
        STZ T5,                                                 ORGLS422
        LXD T4,4                                                ORGLS423
Y4      SXD Y7,1                Y4                              ORGLS424
        CLA 0,2                 Y5                              ORGLS425
        SSP                                                     ORGLS426
        FSB T4                                                  ORGLS427
        TMI Y7                                                  ORGLS428
        CLA 0,2                 Y6                              ORGLS429
        SSP                                                     ORGLS430
        STO T4                                                  ORGLS431
        SXD T5,4                                                ORGLS432
Y7      TIX Y8,2,0              Y7   DEC SET Y4,DELTA           ORGLS433
        HTR Y8                                                  ORGLS434
Y8      TNX Y10,1,1             Y8                              ORGLS435
        TXI Y4,4,1              Y9                              ORGLS436
Y10     CAL T3                  Y10                             ORGLS437
        ADD T2                                                  ORGLS438
        PDX 0,4                                                 ORGLS439
        CLA T5                                                  ORGLS440
        STO 0,4                                                 ORGLS441
        TSX X1,4                Y11                             ORGLS442
        LXD T3,2                Y12                             ORGLS443
        CLA 0,2                                                 ORGLS444
        TZE SING                                                ORGLS445
        TMI SING                                                ORGLS446
        CLA FLONE               Y13                             ORGLS447
```

```
        FDP 0,2                                                    ORGLS448
        STQ 0,2                                                    ORGLS449
        CLS 0,2                                                    ORGLS450
        STO T6                                                     ORGLS451
        CLA PON                 Y14                                ORGLS452
        SUB T3                                                     ORGLS453
        ARS 18                                                     ORGLS454
        STA Y16A                     SETS ADDRESSES                ORGLS455
        STA Y19                         AT M                       ORGLS456
        CLA PON                                                    ORGLS457
        SUB T3                                                     ORGLS458
        ADD T2                                                     ORGLS459
        ARS 18                                                     ORGLS460
        STA Y16                      SETS ADDRESSES                ORGLS461
        STA Y19A                        AT M+N                     ORGLS462
        LXD T2,1                                                   ORGLS463
        LXD T2,2                                                   ORGLS464
        CLA T3                                                     ORGLS465
        SUB T2                                                     ORGLS466
        PDX 0,4                                                    ORGLS467
Y15     TNX Y17,1,1             Y15                                ORGLS468
Y16     LDQ 0,1                 Y16  ADD SET Y14,M+N               ORGLS469
        FMP T6                                                     ORGLS470
        TNO Y16A                                                   ORGLS471
        SXD T12,4                                                  ORGLS472
        TSX OFL,4                                                  ORGLS473
        LXD T12,4                                                  ORGLS474
Y16A    STO 0,1                      ADD SET Y14,M                 ORGLS475
DT1     TNX Y15,0,0                  DEC FOR T1,C(I4)              ORGLS476
Y17     TNX Y24,2,1             Y17                                ORGLS477
        PXD 0,2                 Y18                                ORGLS478
        PDX 0,1                                                    ORGLS479
Y19     LDQ 0,1                 Y19  ADD SET Y14,M                 ORGLS480
Y19A    FMP 0,2                      ADD SET Y14,M+N               ORGLS481
        TNO Y19B                                                   ORGLS482
        SXD T12,4                                                  ORGLS483
        TSX OFL,4                                                  ORGLS484
        LXD T12,4                                                  ORGLS485
```

```
Y19B   FAD 0,4                                                    ORGLS486
       TNO Y19C                                                   ORGLS487
       SXD T12,4                                                  ORGLS488
       TSX OFL,4                                                  ORGLS489
       LXD T12,4                                                  ORGLS490
Y19C   STO 0,4                                                    ORGLS491
       TXI Y20,4,-1                                               ORGLS492
Y20    TNX Y17,1,1          Y20                                   ORGLS493
       TNX Y19,0,0                                                ORGLS494
Y24    LXD T3,2             Y24                                   ORGLS495
       LXD T2,1                                                   ORGLS496
       TNX Y26,1,1                                                ORGLS497
Y25    TIX Y2,2,0           Y25  DEC SET Y2                       ORGLS498
       HTR Y2                                                     ORGLS499
Y26    TXI Y26A,1,1         Y26                                   ORGLS500
Y26A   SXD Y29,1                                                  ORGLS501
Y27    TXL Y29,1,0          Y27  DEC SET Y1,0                     ORGLS502
       LXD T1,4             Y28                                   ORGLS503
       LXD T13,1                                                  ORGLS504
       LXD T14,2                                                  ORGLS505
Y28    STZ 0                ADD SET                               ORGLS506
       EFTM                                                       ORGLS507
       TRA 4,4              NORMAL RETURN                         ORGLS508
Y29    TXI Y29A,2,0         Y29  DEC SET Y26                      ORGLS509
Y29A   SXD T3,2                                                   ORGLS510
       SXD T2,1                                                   ORGLS511
       CLA PON              Y30                                   ORGLS512
       SUB T3                                                     ORGLS513
       ARS 18                                                     ORGLS514
       STA Y35                   SETS ADDRESSES                   ORGLS515
       STA Y38                      AT M                          ORGLS516
       STA Y39                                                    ORGLS517
       STA Y39B                                                   ORGLS518
       STA Y39C                                                   ORGLS519
       CLA PON                                                    ORGLS520
       SUB T3                                                     ORGLS521
       ADD T2                                                     ORGLS522
       ARS 18                                                     ORGLS523
```

```
        STA Y31                     SETS ADDRESSES                  ORGLS524
        STA Y36                        AT M+N                       ORGLS525
        STA Y36A                                                    ORGLS526
        STA Y38B                                                    ORGLS527
        STA Y38C                                                    ORGLS528
        STA Y39A                                                    ORGLS529
        CLA T2                                                      ORGLS530
        SUB ONE                                                     ORGLS531
        PDX 0,1                     SETS INDEXES                    ORGLS532
        PDX 0,2                        AT M-N                       ORGLS533
Y31     STZ 0,1                Y31  ADD SET Y30,M+N                 ORGLS534
        TIX Y31,1,1            Y32                                  ORGLS535
        CLA T3                 Y33                                  ORGLS536
        SUB T2                                                      ORGLS537
        PDX 0,4                                                     ORGLS538
Y34     PXD 0,2                Y34                                  ORGLS539
        PDX 0,1                                                     ORGLS540
Y35     LDQ 0,2                Y35  ADD SET Y30,M                   ORGLS541
        FMP 0,4                                                     ORGLS542
        TNO Y36                                                     ORGLS543
        SXD T12,4                                                   ORGLS544
        TSX OFL,4                                                   ORGLS545
        LXD T12,4                                                   ORGLS546
Y36     FAD 0,1                Y36  ADD SET Y30,M+N                 ORGLS547
        TNO Y36A                                                    ORGLS548
        SXD T12,4                                                   ORGLS549
        TSX OFL,4                                                   ORGLS550
        LXD T12,4                                                   ORGLS551
Y36A    STO 0,1                     ADD SET Y30,M+N                 ORGLS552
        TXI Y37,4,-1                                                ORGLS553
Y37     TNX Y39,1,1            Y37                                  ORGLS554
Y38     LDQ 0,1                Y38  ADD SET Y30,M                   ORGLS555
        FMP 0,4                                                     ORGLS556
        TNO Y38B                                                    ORGLS557
        SXD T12,4                                                   ORGLS558
        TSX OFL,4                                                   ORGLS559
        LXD T12,4                                                   ORGLS560
Y38B    FAD 0,2                     ADD SET Y30,M+N                 ORGLS561
```

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        TNO Y38C                                                ORGLS562
        SXD T12,4                                               ORGLS563
        TSX OFL,4                                               ORGLS564
        LXD T12,4                                               ORGLS565
Y38C    STO 0,2                 ADD SET Y30,M+N                 ORGLS566
        TNX Y35,0,0                                             ORGLS567
Y39     LDQ 0,2                 Y39  ADD SET Y30,M              ORGLS568
Y39A    FMP 0,2                      ADD SET Y30,M+N            ORGLS569
        TNO Y39B                                                ORGLS570
        SXD T12,4                                               ORGLS571
        TSX OFL,4                                               ORGLS572
        LXD T12,4                                               ORGLS573
Y39B    FAD 0                        ADD SET Y30,M              ORGLS574
        TNO Y39C                                                ORGLS575
        SXD T12,4                                               ORGLS576
        TSX OFL,4                                               ORGLS577
        LXD T12,4                                               ORGLS578
Y39C    STO 0                        ADD SET Y30,M              ORGLS579
        TIX Y34,2,1             Y40  GO TO Y50                  ORGLS580
        CAL T3                  Y50                             ORGLS581
        ADD T2                                                  ORGLS582
        PDX 0,4                                                 ORGLS583
        CAL 0,4                                                 ORGLS584
        SLW T5                                                  ORGLS585
        TSX X1,4                Y51                             ORGLS586
        LXD T3,2                Y52                             ORGLS587
        LXD T2,1                                                ORGLS588
DT12    TNX Y26,0,0                  DEC FOR T12                ORGLS589
SING    PXD 0,2                 SINGULARITY RETURN              ORGLS590
        LXD T13,1                                               ORGLS591
        LXD T14,2                                               ORGLS592
        LXD T1,4                                                ORGLS593
        CLA ONE                                                 ORGLS594
SING1   STO 0                   ADD SET                         ORGLS595
        EFTM                                                    ORGLS596
        TRA 4,4                 ERROR RETURN                    ORGLS597
OFL     ARS 1                   OVERFLOW-UNDERFLOW              ORGLS598
        PBT                                                     ORGLS599
```

```
DT13   TNX OFL+5,0,0              DEC FOR T13,C(I1)                ORGLS600
       PXD 0,0,0                                                   ORGLS601
       TRA 1,4                                                     ORGLS602
       PXD 0,4                                                     ORGLS603
       SSM                                                         ORGLS604
DT14   TNX SING+1,0,0             DEC FOR T14,C(I2)                ORGLS605
X1     CLA T5                 X1                                   ORGLS606
       TZE 1,4                                                     ORGLS607
       SXD T12,4              X2                                   ORGLS608
       LXD T2,1                                                    ORGLS609
       LXD T3,2                                                    ORGLS610
       CAL T3                                                      ORGLS611
       SUB T5                                                      ORGLS612
       PDX 0,4                                                     ORGLS613
       STD X6                                                      ORGLS614
X3     CAL 0,2                X3                                   ORGLS615
       LDQ 0,4                                                     ORGLS616
       SLW 0,4                                                     ORGLS617
       STQ 0,2                                                     ORGLS618
       TNX X9,1,1             X4                                   ORGLS619
       SXD X8,1               X5                                   ORGLS620
X6     TXH X8,2,0             X6    DEC SET X2                     ORGLS621
       CAL ONE                X7                                   ORGLS622
       STD X8                                                      ORGLS623
X8     TIX X8A,4,0            X8    DEC SET X5,X7                  ORGLS624
       HTR 0                                                       ORGLS625
X8A    TXI X3,2,-1                                                 ORGLS626
X9     LXD T3,2               X9                                   ORGLS627
       LXD X6,4                                                    ORGLS628
       CAL 0,2                                                     ORGLS629
       LDQ 0,4                                                     ORGLS630
       SLW 0,4                                                     ORGLS631
       STQ 0,2                                                     ORGLS632
       LXD T12,4              X10                                  ORGLS633
       TRA 1,4                                                     ORGLS634
ONE    PZE 0,0,1              ONE                                  ORGLS635
FLONE  DEC 1.0                FLONE                                ORGLS636
PON    PON 0,0,0              LGNO                                 ORGLS637
```

```
T2     PZE 0,0,0              T2, N                                    ORGLS638
T3     PZE 0,0,0              T3,-M                                    ORGLS639
T4     PZE 0,0,0              T4,X    T6,-B11                          ORGLS640
T5     PZE 0,0,0              T5,J                                     ORGLS641
T1     SYN DT1                C(I4)                                    ORGLS642
T6     SYN T4                 -B11                                     ORGLS643
T12    SYN DT12               C(I4) FOR SR                             ORGLS644
T13    SYN DT13               C(I1)                                    ORGLS645
T14    SYN DT14               C(I2)                                    ORGLS646
       END 0                                                           ORGLS647


*TYPE(FORTRAN)                                                         ORGLS648
C      EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTSORGLS649
                                                                       ORGLS650
C      P(1) AND P(2) ARE FIXED PARAMETERS.                             ORGLS651
C      P(1) IS THE X VALUE OF THE FIRST END POINT.                     ORGLS652
C      P(2) IS THE INTERVAL IN X COVERED BY EACH SEGMENT.              ORGLS653
C      P(3),P(4), ETC. ARE THE Y VALUES OF THE END POINTS. THESE       ORGLS654
C         WILL BE ADJUSTED BY LEAST SQUARES.                           ORGLS655
                                                                       ORGLS656
       SUBROUTINE CALC(X,Y,P,D)                                        ORGLS657
                                                                       ORGLS658
       DIMENSION P(10)                                                 ORGLS659
                                                                       ORGLS660
       Z#X-P(1)                                                        ORGLS661
       I#Z/P(2)                                                        ORGLS662
       F#Z/P(2)-FLOATF(I)                                              ORGLS663
       Y#P(I+3)+(P(I+4)-P(I+3))*F                                      ORGLS664
       RETURN                                                          ORGLS665
       END                                                             ORGLS666


*DATA                                                                  ORGLS667
EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.    ORGLS668
  1  6  1  1  1  0  0                                                  ORGLS669
```

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```
  8                                                                                ORGLS670
     10.0      5.0      4.4      5.5      8.4     13.2     16.3     17.3ORGLS671
      4.7               10.8                                                      ORGLS672
      4.7               12.2                                                      ORGLS673
      5.1               13.8                                                      ORGLS674
      5.6               15.6                                                      ORGLS675
      6.5               17.4                                                      ORGLS676
      7.2               18.4                                                      ORGLS677
      8.3               19.8                                                      ORGLS678
      9.9               21.4                                                      ORGLS679
     10.4               22.2                                                      ORGLS680
     12.1               24.0                                                      ORGLS681
     13.4               25.2                                                      ORGLS682
     15.1               27.2                                                      ORGLS683
     15.9               28.8                                                      ORGLS684
     16.2               30.0                                                      ORGLS685
     17.0               32.2                                                      ORGLS686
     17.1               34.2                                                      ORGLS687
1                                                                                  ORGLS688
00111111                                                                           ORGLS689
        0        0      0.01     0.01     0.01     0.01     0.01     0.01ORGLS690
```

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```
EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

NUMBER OF CYCLES IN THIS JOB IS 1

NUMBER OF PARAMETERS TO BE VARIED IS  6

NUMBER OF INDEPENDENT VARIABLES PER OBSERVATION IS 1

NUMERICAL DERIVATIVES UNLESS PARAMETER INCREMENT IS ZERO

UNIT WEIGHTS TO BE SET BY PROGRAM

PARAMETERS TO BE READ AS INPUT DATA

CORRECTED PARAMETERS NOT TO BE SAVED FOR LATER USE

NUMBER OF PARAMETERS READ IS  8

NUMBER OF OBSERVATIONS READ IS  16

INPUT DATA

  I      P(I)  KI(I)      DP(I)

  1    10.0000   0     0.
  2     5.0000   0     0.
  3     4.4000   1     1.0000E-02
  4     5.5000   1     1.0000E-02
  5     8.4000   1     1.0000E-02
  6    13.2000   1     1.0000E-02
  7    16.3000   1     1.0000E-02
  8    17.3000   1     1.0000E-02
```

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 1

Y(OBS)	Y(CALC)	OBS-CALC	SIG(O)	(O-C)/SIG(O)	X(I)
4.7000	4.5760	0.1240	1.0000	0.1240	10.8000
4.7000	4.8840	-0.1840	1.0000	-0.1840	12.2000
5.1000	5.2360	-0.1360	1.0000	-0.1360	13.8000
5.6000	5.8480	-0.2480	1.0000	-0.2480	15.6000
6.5000	6.8920	-0.3920	1.0000	-0.3920	17.4000
7.2000	7.4720	-0.2720	1.0000	-0.2720	18.4000
8.3000	8.2840	0.0160	1.0000	0.0160	19.8000
9.9000	9.7440	0.1560	1.0000	0.1560	21.4000
10.4000	10.5120	-0.1120	1.0000	-0.1120	22.2000
12.1000	12.2400	-0.1400	1.0000	-0.1400	24.0000
13.4000	13.3240	0.0760	1.0000	0.0760	25.2000
15.1000	14.5640	0.5360	1.0000	0.5360	27.2000
15.9000	15.5560	0.3440	1.0000	0.3440	28.8000
16.2000	16.3000	-0.1000	1.0000	-0.1000	30.0000
17.0000	16.7400	0.2600	1.0000	0.2600	32.2000
17.1000	17.1400	-0.0400	1.0000	-0.0400	34.2000

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 0.9042E 00

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.3007

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

	OLD	CHANGE	NEW	ERROR
1	10.0000		10.0000	
2	5.0000		5.0000	
3	4.4000	0.1615	4.5615	0.2275
4	5.5000	-0.3648	5.1352	0.1767
5	8.4000	-0.0886	8.3114	0.1489
6	13.2000	0.1295	13.3295	0.1552
7	16.3000	0.2280	16.5280	0.1588
8	17.3000	-0.0067	17.2933	0.2372

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

SUM(W*(O-C)**2) IS 0.4651E-00

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.2157

EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 2

Y(OBS)	Y(CALC)	OBS-CALC	SIG(O)	(O-C)/SIG(O)	X(I)
4.7000	4.6533	0.0467	1.0000	0.0467	10.8000
4.7000	4.8139	-0.1139	1.0000	-0.1139	12.2000
5.1000	4.9975	0.1025	1.0000	0.1025	13.8000
5.6000	5.5163	0.0837	1.0000	0.0837	15.6000
6.5000	6.6598	-0.1598	1.0000	-0.1598	17.4000
7.2000	7.2950	-0.0950	1.0000	-0.0950	18.4000
8.3000	8.1843	0.1157	1.0000	0.1157	19.8000
9.9000	9.7164	0.1836	1.0000	0.1836	21.4000
10.4000	10.5193	-0.1193	1.0000	-0.1193	22.2000
12.1000	12.3258	-0.2258	1.0000	-0.2258	24.0000
13.4000	13.4574	-0.0574	1.0000	-0.0574	25.2000
15.1000	14.7368	0.3632	1.0000	0.3632	27.2000
15.9000	15.7604	0.1396	1.0000	0.1396	28.8000
16.2000	16.5280	-0.3280	1.0000	-0.3280	30.0000
17.0000	16.8647	0.1353	1.0000	0.1353	32.2000
17.1000	17.1709	-0.0709	1.0000	-0.0709	34.2000

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 2

SUM(W*(O-C)**2) IS 0.4651E-00

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.2157

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EXAMPLE. FITTING A CURVE WITH A SEQUENCE OF STRAIGHT LINE SEGMENTS.

CORRELATION MATRIX

1	1.0000	-0.4062	0.1268	-0.0353	0.0083	-0.0023
2	0.	1.0000	-0.3120	0.0869	-0.0204	0.0058
3	0.	0.	1.0000	-0.2787	0.0652	-0.0185
4	0.	0.	0.	1.0000	-0.2341	0.0664
5	0.	0.	0.	0.	1.0000	-0.2836
6	0.	0.	0.	0.	0.	1.0000

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OR FLS, A Fortran crystallographic least-squares program, ORNL-TM-305, Oak Ridge, TN : Oak Ridge National Laboratory, 1962.

by W. R. Busing, K. O. Martin, and H. A. Levy

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ORNL-TM-305

OR FLS,

A FORTRAN CRYSTALLOGRAPHIC LEAST-SQUARES PROGRAM

W. R. Busing
K. O. Martin
H. A. Levy

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OR FLS,

A FORTRAN CRYSTALLOGRAPHIC LEAST-SQUARES PROGRAM

by

W. R. Busing, K. O. Martin, and H. A. Levy
Chemistry Division and Mathematics Division

August, 1962

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ABSTRACT

This report describes a computer program to perform the least-squares refinement of crystal structure parameters based on x-ray or neutron diffraction measurements. The program is written mostly in the Fortran language to facilitate modification and to permit its use on various machines. Detailed instructions for its use are included, and the required card decks may be obtained from the authors.

INTRODUCTION

This report describes a computer program to perform the least-squares refinement of crystal structure parameters based on x-ray or neutron diffraction measurements. Detailed instructions for its use are included, and the required card decks may be obtained from the authors.

The program performs successive cycles of refinement using the full matrix of the normal equations. The parameters which may be adjusted include several scale factors, an over-all temperature factor coefficient, the neutron scattering factors, individual atom multipliers, atomic coordinates, and isotropic or anisotropic individual atom temperature factor coefficients. The parameters to be varied may be specified arbitrarily, and structures of any symmetry may be accommodated. The refinement may be based either on the structure factors or their squares, and the observations may be weighted individually, or the use of unit weights may be specified.

The program is mathematically similar to an earlier version, OR XLS (W. R. Busing and H. A. Levy, "A Crystallographic Least Squares Refinement Program for the IBM 704," ORNL-CF 59-4-37, 1959). A basic difference is that the present program is not segmented and does not use magnetic tape for intermediate storage. This implies that a 32k core memory will be required for most problems. A means of expanding the storage capacity with magnetic tape is

mentioned briefly in a later section. Provision is made to transfer parameters from one job to the next by means of magnetic tape or punched cards.

The present program is derived from a general least-squares program (W. R. Busing and H. A. Levy, "OR GLS, A General Fortran Least Squares Program," ORNL-TM-271, 1962), and programmers contemplating extensive changes should consider starting with that basic program.

In order to facilitate modification of the program and to permit its use on various machines, OR FLS has been written in the Fortran language except for the matrix inverter which is in FAP suitable for the IBM 704, 709, or 7090. A test problem is provided to serve as an example and to aid in checking the program at other installations.

GENERAL DESCRIPTION

It is expected that the Fortran listing and the glossary of symbols which are provided will serve as a complete description of the program. The form of the input is described in detail in a separate section, and an example of such input, together with the corresponding output, is also given. This section, therefore, is intended to serve only as a summary of the method.

Because the present routine is a modification of the general least-squares program, OR GLS, it was convenient to divide it into several subprograms. The main program performs the basic operations associated with the least-squares

refinement, while subroutine PRELIM serves to read the control information and parameters which define the trial crystal structure. Subroutine CALC computes the scaled structure factors or their squares and the derivatives of these quantities with respect to the trial parameters, and subroutine TEST determines whether the adjusted temperature factor coefficients are positive-definite.

In the calculation of the structure factors and their derivatives it is useful to distinguish the different types of parameters such as scale factors, coordinates, and temperature factor coefficients and to store them in separate arrays. For the least-squares adjustment procedure, however, it is more convenient to store all the parameters in a single array. To achieve both of these objectives the program uses duplicate storage arrays for the crystal structure parameters, and subroutine PTOSB is provided to copy them from the array P to the various storage locations SC, TO, SF, AI, XYZ, and BETA. Subroutine SBTOP performs the reverse information transfer and is also used to execute an analogous operation with the calculated derivatives.

The sequence of operations begins with the reading of all the input data. This is performed partly by the main program and partly by subroutine PRELIM. Most of the items read are immediately put out by the program to aid in diagnosing difficulties.

If the control card indicates that isotropic temperature

factor coefficients, T_i, are to be converted to anisotropic form, subroutine **PRELIM** computes for each atom

$$\beta_{11_i} = T_i a^{*2}/4,$$

$$\beta_{12_i} = T_i a^* b^* \cos\gamma^*/4,$$

etc.

Here the β's are the anisotropic temperature factor coefficients defined in the next section, and a*, b*, ..., γ* are the reciprocal cell parameters. The program then proceeds as though anisotropic coefficients had been read.

For each cycle the matrix and vector of the normal equations are stored by computing the contributions of one observation at a time. For this purpose subroutine CALC is entered once for each reflection to obtain YC, the calculated absolute value of the scaled structure factor or its square. CALC also stores in the array DC the derivatives of YC with respect to all parameters, P, whether they are to be varied or not. The expressions for these quantities are summarized in the following table, in which F is the magnitude of the structure factor, s_q is the scale factor, T_o is the over-all temperature factor coefficient, ρ is $\sin^2\theta/\lambda^2$, A and B are the real and imaginary components of the structure factor, and p is any individual atom parameter.

	Centrosymmetric with origin at symmetry center	Non-centrosymmetric
(s_qF)	$2s_q \exp(-T_o\rho)\lvert A\rvert$	$s_q \exp(-T_o\rho)(A^2 + B^2)^{1/2}$
$\partial(s_qF)/\partial s_q$	$(s_qF)/s_q$	$(s_qF)/s_q$
$\partial(s_qF)/\partial T_o$	$-\rho(s_qF)$	$-\rho(s_qF)$
$\partial(s_qF)/\partial p$	$2s_q \exp(-T_o\rho)(\partial\lvert A\rvert/\partial p)$	$s_q \exp(-T_o\rho)(A^2 + B^2)^{-1/2} \cdot [A(\partial A/\partial p) + B(\partial B/\partial p)]$
$(s_qF)^2$	$4s_q^2 \exp(-2T_o\rho)A^2$	$s_q^2 \exp(-2T_o\rho)(A^2 + B^2)$
$\partial(s_qF)^2/\partial s_q$	$2(s_qF)^2/s_q$	$2(s_qF)^2/s_q$
$\partial(s_qF)^2/\partial T_o$	$-2\rho(s_qF)^2$	$-2\rho(s_qF)^2$
$\partial(s_qF)^2/\partial p$	$8s_q^2 \exp(-2T_o\rho)A(\partial A/\partial p)$	$2s_q^2 \exp(-2T_o\rho) \cdot [A(\partial A/\partial p) + B(\partial B/\partial p)]$

The expressions for A and B and their derivatives are summarized in the following table. Here the subscripts i and j refer to the various atoms in the asymmetric unit and to the different equivalent positions, respectively. T_i, f_i, and a_i are the isotropic temperature factor coefficient, scattering factor, and scattering factor multiplier, respectively, for atom i. The terms $\cos_{ij}$, $\sin_{ij}$, and $\exp_{ij}$ are the trigonometric contributions and the anisotropic temperature factor of atom i in equivalent position j. The expressions h_j and $(2hk)_j$ are representative of the transformed indices and index products. These terms are discussed in detail in the next section.

	Isotropic temperature factor	Anisotropic temperature factor
A	$\sum_i f_i a_i \exp(-T_i\rho) \sum_j \cos_{ij}$	$\sum_i f_i a_i \sum_j \exp_{ij} \cos_{ij}$
B	$\sum_i f_i a_i \exp(-T_i\rho) \sum_j \sin_{ij}$	$\sum_i f_i a_i \sum_j \exp_{ij} \sin_{ij}$
$\partial A/\partial f_i$	$a_i \exp(-T_i\rho) \sum_j \cos_{ij}$	$a_i \sum_j \exp_{ij} \cos_{ij}$
$\partial B/\partial f_i$	$a_i \exp(-T_i\rho) \sum_j \sin_{ij}$	$a_i \sum_j \exp_{ij} \sin_{ij}$
$\partial A/\partial a_i$	$f_i \exp(-T_i\rho) \sum_j \cos_{ij}$	$f_i \sum_j \exp_{ij} \cos_{ij}$
$\partial B/\partial a_i$	$f_i \exp(-T_i\rho) \sum_j \sin_{ij}$	$f_i \sum_j \exp_{ij} \sin_{ij}$
$\partial A/\partial T_i$	$-\rho f_i a_i \exp(-T_i\rho) \sum_j \cos_{ij}$	-----
$\partial B/\partial T_i$	$-\rho f_i a_i \exp(-T_i\rho) \sum_j \sin_{ij}$	-----
$\partial A/\partial x_i$	$-2\pi f_i a_i \exp(-T_i\rho) \sum_j h_j \sin_{ij}$	$-2\pi f_i a_i \sum_j h_j \exp_{ij} \sin_{ij}$
$\partial B/\partial x_i$	$2\pi f_i a_i \exp(-T_i\rho) \sum_j h_j \cos_{ij}$	$2\pi f_i a_i \sum_j h_j \exp_{ij} \cos_{ij}$
$\partial A/\partial B_{12i}$	-----	$-f_i a_i \sum_j (2hk)_j \exp_{ij} \cos_{ij}$
$\partial B/\partial \beta_{12i}$	-----	$-f_i a_i \sum_j (2hk)_j \exp_{ij} \sin_{ij}$

The program does the computation for each reflection in three steps. First the sums over j are accumulated. These are then converted to the derivatives of A and B with respect to the atomic parameters, and A and B are obtained. Finally, the scaled structure factor or its square and the derivatives of this quantity are computed.

Upon return from subroutine CALC, a line of output comparing the observation with its calculated value is put out. The term (SQRTW*DV(J))*(SQRTW*DV(K)) is then added to AM(JK), the J,Kth element of the matrix, where SQRTW is the square root of the weight of the observation. The contribution to the vector element V(J) is (SQRTW*DV(J))*(SQRTW*(YO-YC)), and that to the agreement factor SIG is (SQRTW*(YO-YC))**2. Here YO is used as an abbreviation for YO(I), the Ith observed value of $|F|$ or F^2.

The sums involved in the following unweighted and weighted R factors are accumulated both for all observations and for non-zero observations.

	Refining on $\|F\|$	Refining on F^2
R	$\Sigma\|F_o - s_qF\|/\Sigma\|F_o\|$	$\Sigma\|F_o^2 - (s_qF)^2\|/\Sigma\|F_o^2\|$
Weighted R	$\sqrt{\Sigma w(F_o - s_qF)^2}/\sqrt{\Sigma wF_o^2}$	$\sqrt{\Sigma w(F_o^2 - (s_qF)^2)^2}/\sqrt{\Sigma w(F_o^2)^2}$

The calculation of YC and its derivatives is repeated until the contributions from all the observations have been obtained. At this point an agreement factor, the standard error of an observation of unit weight, SQRTF(SIG/(NO-NV)), is computed and put out together with the R factors.

The storage scheme used for the matrix AM is described in the glossary. To make efficient use of memory space,

only the upper triangular part of this symmetric matrix is stored. Furthermore, to conform to the requirements of the existing matrix inverter, SMI, the matrix is stored forward in core or backward in the normal Fortran indexing system.

Before the matrix is inverted it is tested for zero diagonal elements, which would indicate a singular matrix with one or more zero row-columns. This would be the result if the derivatives with respect to the corresponding parameters were zero for all observations. A singular matrix due to the attempt to vary sets of parameters with one or more redundancies will be found in the course of the inversion. In case of either type of singularity, the job is terminated with the appropriate comment.

The matrix inversion procedure is described in detail elsewhere (W. R. Busing and H. A. Levy, "A Procedure for Inverting Large Symmetric Matrices," Comm. ACM (Aug. 1962) 5 445-446). It involves the diagonalization of the matrix by a series of congruent transformations, inversion by taking reciprocals of the diagonal elements, and a sequence of reverse transformations. Upon completion of the process the inverse matrix has replaced the original one in the array AM.

The vector is then multiplied by the inverse matrix to obtain the parameter changes, PD. An estimated new value of the agreement factor SIG is obtained by subtracting from it PD(I)*V(I) summed over the NV variables, and a revised SQRTF(SIG/(NO-NV)) is computed. The entire list of parameters is then put out showing the changes which were made and the

estimated standard errors associated with these variables. The latter are computed as SQRTF(DIAG(J)*SIG/(NO-NV)), where DIAG is an array of the diagonal elements of the inverse matrix. It should be noted that these estimates are approximately correct if the refinement is converging but may be grossly incorrect if the calculation is diverging.

The program then calls subroutine TEST to examine the new temperature factor coefficients. If the over-all temperature factor T_o is not zero, it is added to the individual atom temperature factors so that $T_i' = T_i + T_o$ for isotropic temperature factors or

$$\beta_{11}' = \beta_{11} + T_o\ a^{*2}/4,$$

$$\beta_{12}' = \beta_{12} + T_o\ a^*b^*\cos\gamma^*/4,$$

etc.,

for anisotropic temperature factors. T_o is then set to zero. These operations are performed so that the temperature factor coefficients may be tested for positive-definite form in the following way. For isotropic temperature factors:

$$T_i \geqslant 0.$$

For anisotropic temperature factors:

$$\beta_{11} \geqslant 0,\ \beta_{22} \geqslant 0,\ \beta_{33} \geqslant 0,$$

$$\begin{vmatrix} \beta_{22} & \beta_{23} \\ \beta_{23} & \beta_{33} \end{vmatrix} \geqslant 0,\quad \begin{vmatrix} \beta_{11} & \beta_{13} \\ \beta_{13} & \beta_{33} \end{vmatrix} \geqslant 0,\quad \begin{vmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{vmatrix} \geqslant 0,$$

$$\begin{vmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & \beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{vmatrix} \geqslant 0.$$

Failure of one of these tests means that the coefficients do not represent physical reality. In this case an indicator is set to terminate the job, and a statement is put out describing the error.

Upon return from TEST, if the control integer IT $\neq$ 0, the new parameters are put out on an auxiliary magnetic tape in the same format as the parameter input. This tape may be used to punch cards for input to future jobs, or the tape itself may serve as this input.

Unless the job is ended by TEST or unless a singular matrix has been found, the least-squares procedure will be repeated for the specified number of cycles, and then a final calculation and output of s_qF or $(s_qF)^2$ will be made.

If a singular matrix has not been found, the program computes the correlation matrix by dividing each inverse matrix element AM(IJ) by SQRTF(DIAG(I)*DIAG(J)) when the refinement is terminated. Only the upper triangular part of this symmetric matrix is reported, and the other elements appear as zero in the listing.

At the end of the job, if the control integer IXFE = 1, and if the matrix is not singular, a tape is written for use by the function and error program, OR FFE . (W. R. Busing, K. O. Martin, and H. A. Levy, "OR FFE, A Fortran Crystallographic Function and Error Program," ORNL-TM-306, 1962). This tape includes the final parameters, the variance-covariance matrix, and other quantities needed for the calculation of interatomic distances, angles, principal

thermal displacements, etc., and the standard errors of these quantities.

SYMMETRY CONSIDERATIONS

In the expressions for A and B, the terms $\cos_{ij}$ and $\sin_{ij}$ are the trigonometric contributions of the ith atom transformed to the jth equivalent position, and $\exp_{ij}$ is the anisotropic temperature factor for this atom. **OR FLS** sets either $\exp(-T_i\rho)$ or $\exp_{ij}$ to unity, depending on the kind of temperature factor to be used.

The trigonometric contribution $\cos_{ij}$ could be computed as

$$\cos_{ij} = \cos 2\pi(hx_{ij} + ky_{ij} + \ell z_{ij}).$$

Here h, k, and ℓ are the indices and x_{ij}, y_{ij}, and z_{ij} are the coordinates of the ith atom in the asymmetric unit transformed to the jth equivalent position. **OR FLS** does not do this, however. Instead of transforming the coordinates, the indices h, k, and ℓ are transformed in a way which makes the result identical with the above:

$$\cos_{ij} = \cos 2\pi(h_j x_i + k_j y_i + \ell_j z_i + t_j).$$

Here x_i, y_i, and z_i are the (untransformed) coordinates for the ith atom in the asymmetric unit; h_j, k_j, and ℓ_j are the transformed indices; and t_j is a translational term. As an example, we will illustrate the transformations used for the general positions of space group $P3_22$. Substitution of these quantities in the two expressions for $\cos_{ij}$ will give identical results. The expression for $\sin_{ij}$ is obtained in an analogous way.

j	x_j	y_j	z_j	h_j	k_j	ℓ_j	t_j
1	x	y	z	h	k	ℓ	0
2	x-y	-y	-z	h	-h-k	$-\ell$	0
3	y-x	-x	1/3 + z	-h-k	h	ℓ	$\ell/3$
4	-x	y-x	1/3 - z	-h-k	k	$-\ell$	$\ell/3$
5	-y	x-y	2/3 + z	k	-h-k	ℓ	$2\ell/3$
6	y	x	2/3 - z	k	h	$-\ell$	$2\ell/3$

OR FLS permits any desired symmetry to be introduced by means of symmetry cards included as input data. There is one such card for each j value, and it consists of a statement of the coordinate transformations (as in the left half of the above table). The program automatically transforms the indices in ways which are equivalent to the coordinate transformations specified.

The anisotropic temperature factor, $\exp_{ij}$, is handled similarly. The fundamental expression is

$$\exp_{ij} = \exp\{-[h^2\beta_{11_{ij}} + k^2\beta_{22_{ij}} + \ell^2\beta_{33_{ij}} + 2hk\beta_{12_{ij}} + 2h\ell\beta_{13_{ij}} + 2k\ell\beta_{23_{ij}}]\}$$

where $\beta_{11_{ij}}$, etc., are the six temperature factor coefficients for the ith atom of the asymmetric unit transformed to the jth equivalent position. Again the program makes the computation by transforming the index products rather than the coefficients themselves so that

$$\exp_{ij} = \exp\{-[(h^2)_j\beta_{i}^{11} + (k^2)_j\beta_{i}^{22} + (\ell^2)_j\beta_{i}^{33} + (2hk)_j\beta_{i}^{12} + (2h\ell)_j\beta_{i}^{13} + (2k\ell)_j\beta_{i}^{23}]\}.$$

Here $(h^2)_j$, etc., are the transformed index products which make the two expressions identical.

Rules for obtaining the transformed coefficients β_{ij}^{11}, etc., for any space group have been given by H. A. Levy (Acta Cryst. (1956) 9, 679). From these rules it may be deduced that for atoms in general positions $(h^2)_j = (h_j)^2$, etc., so that the transformed index products are simply the products of the transformed indices. This is not necessarily true for atoms in special positions, however. **OR FLS** computes the products of transformed indices and assumes that $(h^2)_j = (h_j)^2$, etc., and therefore the computed anisotropic temperature factor may not be valid for atoms in special positions.

Cells with translational symmetry (centering)

The specification of symmetry in the case of face-centered, end-centered, or body-centered cells can be simplified (and the computing time reduced) provided that the reflections which are extinguished by centering are not computed. Similar considerations apply to a rhombohedral cell described by hexagonal coordinates. In these cases, symmetry cards need be supplied only for positions not related by translation. The atom multipliers should then be increased by the appropriate factor.

Special positions

The ways of performing the computation when atoms are in special positions will now be considered. The important effects of atoms being in special positions are (a) that the number of these atoms is smaller than if they were in general positions, (b) that there are certain restrictions on the position parameters, and (c) that there may be some restrictions on the anisotropic temperature factor coefficients. No restrictions on isotropic temperature factors are introduced, however.

The ways of treating special positions with **OR FLS** depend on several factors: (1) whether all the atoms are in the same kind of special position, (2) whether the position parameters have a fixed value or whether there is a relationship among two or more coordinates, (3) whether anisotropic temperature factors are used or not, and (4) if they are used, whether there are (a) no restrictions on the coefficients, (b) certain coefficients fixed at zero, or (c) a relationship between two or more coefficients. H. A. Levy (loc. cit.) has given a rule for determining the restrictions on the anisotropic temperature factor coefficients of atoms in special positions.

Fixed parameters. When coordinates or temperature factor coefficients have fixed values, these values may be put into the list of trial parameters, and the parameter selection cards are prepared so that these parameters are not varied.

Symmetry cards for the general positions are used so that anisotropic temperature factors are correctly computed.

Symmetry cards for special positions. If all atoms are in the same kind of special position, and if anisotropic temperature factors are not used, then the correct result will be obtained by using symmetry cards for the special positions. For example, the space group $P3_2 2$ mentioned above has special positions for y = x, z = 1/3 with the transformations:

j	x_j	y_j	z_j
1	x	x	1/3
2	0	-x	2/3
3	-x	0	0

This information can be introduced with three symmetry cards instead of using six for the general positions. All coordinates y and z in the parameter input are then irrelevant, and no attempt may be made to vary them.

Writing a special subroutine. It is possible to treat any symmetry situation which can arise by using symmetry cards for the general positions, allowing the program to compute the transformed indices and the index products which would be valid for these general positions, and then causing the program to modify these transformed indices appropriately by means of a specially prepared subroutine. Consider, for

example, the special positions mentioned above. The basic program alone would produce the trigonometric argument

$$h_j x_i + k_j y_i + \ell_j z_i + t_j .$$

If x_i is assumed to be the independent variable, then $y_i = x_i$ and $z_i = 1/3$. Substituting these in the argument yields

$$h_j x_i + k_j x_i + \ell_j/3 + t_j .$$

The program will produce this result if a subroutine is provided to replace h_j by $h_j' = h_j + k_j$, k_j by $k_j' = 0$, ℓ_j by $\ell_j' = 0$, and t_j by $t_j' = t_j + \ell_j/3$. The parameters y and z will again be irrelevant and must not be varied.

The restrictions on the anisotropic temperature factor coefficients may be handled in a similar way. For the atoms in the above example, Levy's rule shows that $\beta_{22} = \beta_{11}$, $\beta_{23} = -\beta_{13}$. Taking β_{11} and β_{13} as independent, the transformations to be performed by the subroutine are:

$$\begin{aligned}
(h^2)_j' &= (h^2)_j + (k^2)_j \\
(k^2)_j' &= 0 \\
(\ell^2)_j' &= (\ell^2)_j \\
(2hk)_j' &= (2hk)_j \\
(2h\ell)_j' &= (2h\ell)_j - (2k\ell)_j \\
(2k\ell)_j' &= 0 .
\end{aligned}$$

In this case β_{22} and β_{23} are irrelevant and must not be varied.

One subroutine named PATCH may be prepared by the user to transform both the indices and the index products. Specifications for this subprogram are given below.

Although the parameters y, β_{22}, and β_{23} in the above

example are irrelevant, it may be desirable to reset y = x, $\beta_{22} = \beta_{11}$, and $\beta_{23} = -\beta_{13}$ at the end of each cycle. In the case of the anisotropic temperature factor coefficients, this is necessary if the test for positive-definite form is to be valid. To provide for such resetting, the program calls two subroutines named RESETX and RESETB which may be prepared by the user according to specifications given below.

There is no reason why a combination of the fixed parameter and special subroutine methods may not be used. In the above example the z parameters could be fixed at 1/3 while the subroutine provides for the restriction, y = x. It may also be possible to choose a coordinate system which simplifies the restrictions on the parameters.

Correcting the number of atoms. The program as written always sums over all the equivalent positions specified by the symmetry cards. Thus the effective number of times an atom is included is equal to the number of symmetry cards for non-centrosymmetric structures and twice that number for centrosymmetric structures. If the symmetry cards describe the general positions, then atoms in special positions may be put in correctly by using the appropriate atom multiplier. When the symmetry cards are written for the special positions directly, an atom multiplier of unity will usually be correct.

SPECIFICATIONS FOR SUBROUTINES

This section will give the specifications for the three subroutines which may be needed when atoms are in special positions. The purpose of these subprograms has been discussed in the previous section, and examples of such routines are included in the test problem which is provided. This problem is a hypothetical one based on alpha quartz with space group $P3_2 2$, and the general and special positions used as examples earlier correspond to the positions of oxygen and silicon atoms, respectively.

PATCH(I,TJ,HJ,HHJ)

In the calculation of one structure factor, this routine will be called NA times for each of the NS symmetry positions. On each entry the argument I defines the atom which is being considered so that I = 1,2,....,NA on successive entries for a given symmetry position.

The remaining arguments represent the transformed indices and index products as described in the glossary. On the first entry for each symmetry position, that is, for I = 1, these arguments will have been set by the program according to the information on one symmetry card. It is the task of this subroutine to modify these quantities appropriately. On successive entries for the same symmetry position these arguments will retain the values set previously by the subroutine. The main program does not reset them until it advances to a new symmetry position.

The array HHJ is irrelevant when isotropic temperature factors are used, so that no difficulty will be incurred by including a subroutine prepared for the anisotropic case in an isotropic refinement.

The statements required may be outlined as follows:

```
SUBROUTINE PATCH(I,TJ,HJ,HHJ)
DIMENSION HJ(3), HHJ(6)

Interrogate I with one or more IF statements to
determine whether the values of the arguments are
to be modified.

Set the values of the arguments appropriately.

RETURN
END
```

The subroutine should be compiled and substituted for the dummy program which is included with the card deck provided.

RESETX(XYZ)

This subroutine is called once near the end of each cycle of least squares. It is entered after the main output of the adjusted parameters but before the auxiliary output on cards or tape.

The array XYZ contains the atomic coordinates as described in the glossary. The statements to be included may be summarized as follows:

```
SUBROUTINE RESETX(XYZ)
DIMENSION XYZ(3,20)

Set the values of the constrained coordinates equal
to the appropriate functions of the parameters which
have been adjusted.

RETURN
END
```

The subroutine should be compiled and substituted for the dummy program which is included with the card deck provided.

RESETB(BETA)

This subroutine is called once near the end of each cycle except that it is not called when isotropic temperature factors are used. It is entered after the main output of the adjusted parameters but before the tests for positive-definite form and before the auxiliary output on cards or tape.

The array BETA contains the anisotropic temperature factor coefficients as described in the glossary. The statements to be included may be summarized as follows:

```
SUBROUTINE RESETB(BETA)
DIMENSION BETA(6,20)

Set the values of the constrained coefficients equal
to the appropriate functions of those which have been
adjusted.
```

```
RETURN
END
```

The subroutine should be compiled and substituted for the dummy program which is included with the card deck provided.

POSSIBLE CAUSES OF A SINGULAR MATRIX

A singular matrix may be the result of one of several kinds of errors in the input data. When one or more zero diagonal elements are found in the original matrix, the following sources of error should be considered:

1) Attempting to vary some undetermined parameter, for example, a z-coordinate, when only hk0 data are used.

2) Attempting to vary a parameter which should be fixed because an atom is in a special position.

A singular matrix with no zero diagonal elements may be the result of one of the following errors:

3) Attempting to vary more parameters than there are observations. An error in weighting could cause this difficulty.

4) Attempting to vary redundant parameters such as the over-all temperature factor and all the individual atom temperature factors, or the coordinates of all atoms when the origin is not fixed by the symmetry.

The singularity without zero diagonal elements is more difficult to diagnose. If other approaches fail, the redundant parameters can always be identified by trying refinements with various parameters held constant.

In either case, the output of the trial parameters and parameter selection integers should be checked, as the difficulty may simply be the result of a mistake on these input cards.

CAPACITY AND ARRAY DIMENSIONS

The user may wish to recompile the program with modified DIMENSION statements in order to allocate storage for a particular problem. The following table illustrates the way in which the storage used by the arrays depends on the different variables. The figures included correspond to the dimensions in the program as distributed.

Maximum Values		Storage Used	
NV	100	5*NV + NV*(NV + 3)/2	5650
NP	230	3*NP	690
NO	2500	6*NO	15000
NA	20	45*NA	900
NQ	9	2*NQ	18
NF	10	32*NF	320
NS	24	9*NS	216
		Total	22794

The number of locations occupied by the complete program with temporary storage not listed above is about 6500. This

leaves approximately 3400 locations for use by the monitor system, for subroutines added by the user, or for expansion of the capacity of the program.

For large problems a simple modification may be made which will remove all restrictions from NO and allow NV to increase to about 200. Since the observations are used one at a time, the values of X, YO, and SIGYO may be written on magnetic tape at input time, one observation to a record, and read back for use during the loop through the observations.

Another approach to large problems would be to vary different blocks of parameters successively. For this purpose the user may wish to modify the program to read parameter selection cards at the beginning of each cycle.

DATA INPUT

The limitations marked with an asterisk (*) depend only on the dimensions with which the program is compiled.

1. Title card. FORMAT(12A6)

Columns	
1-72	Title consisting of any desired Hollerith information. This will be put out as a heading on each section of output.

2. Control cards. First card FORMAT(6I3)

Columns	
1-3	NC, the number of cycles to be run on this job. Calculated values of YC, the scaled structure factor or its square, will be listed NC + 1 times. If NC = 0, one list of YC will be put out, but no refinement will be made.
4-6	NV, the number of parameters to be varied. If NC = 0, then NV is irrelevant. $1 \leqslant NV \leqslant 100$.*

Columns	
7-9	IW, the weight indicator. IW = 0 indicates that individual standard errors will be supplied by the user for each observation. IW = 1 indicates that the program is to weight each observation at unity.
10-12	IP, the parameter input indicator. If IP = 0, the trial parameters P are to be read as input data. If IP > 0, then the parameters are to be taken from the magnetic tape output of cycle IP of a previous job.
13-15	IT, the parameter output indicator. If IT = 0, parameters are not to be written on tape for use as input to later least-squares cycles. If IT = 1, they are to be written on a private tape. If IT = 2, they are written on the monitor auxiliary tape in such a way as to yield punched cards. The private tape is initially rewound and is terminated by an end-of-file while the auxiliary tape is not.
16-18	IXFE, the function and error output indicator. If IXFE = 1, information including the parameters and the variance-covariance matrix will be written on a private tape for use by OR FFE. If IXFE = 0, no such output will be made.

Second card FORMAT(7I3)

Columns	
1-3	IFSQ, the F^2 indicator. If IFSQ = 1, the program calculates s_qF. If IFSQ = 2, the program calculates $(s_qF)^2$.
4-6	ITF, the temperature factor indicator. ITF = 1 for isotropic temperature factors. ITF = 2 for anisotropic temperature factors. If ITF = 3, the program converts isotropic temperature factor coefficients to anisotropic form before refining.
7-9	NF, the number of different x-ray form factor tables to be used. For neutron diffraction NF = 0. $0 \leqslant NF \leqslant 10$.*
10-12	NA, the number of atoms in the asymmetric unit. $1 \leqslant NA \leqslant 20$.*

Columns	
13-15	ICENT, the symmetry indicator. ICENT = 1 indicates a centrosymmetric structure with the origin at a symmetry center. ICENT = 2 indicates a non-centrosymmetric structure.
16-18	NS, the number of symmetry cards. For non-centrosymmetric structures NS is equal to the number of equivalent positions. For centrosymmetric structures NS is equal to one-half the number of equivalent positions. $1 \leqslant NS \leqslant 24$.*
19-21	NQ, the number of scale factors in the parameter list. $1 \leqslant NQ \leqslant 9$.*

3. Scattering factor tables. FORMAT(8F9.3)
Four cards are to be provided for each of NF tables. For neutron diffraction problems NF = 0, and these cards are omitted. Entries beyond the range needed for linear interpolation may be left blank.

First card Columns	
1-9	Scattering factor for $\sin\theta/\lambda = 0.00$
10-18	Scattering factor for $\sin\theta/\lambda = 0.05$
.	.
.	.
.	.
64-72	Scattering factor for $\sin\theta/\lambda = 0.35$
Second card Columns	
1-9	Scattering factor for $\sin\theta/\lambda = 0.40$
.	.
.	.
.	.
Third card Columns	
1-9	Scattering factor for $\sin\theta/\lambda = 0.80$
.	.
.	.
.	.
Fourth card Columns	
1-9	Scattering factor for $\sin\theta/\lambda = 1.20$
.	.
.	.
.	.
64-72	Scattering factor for $\sin\theta/\lambda = 1.55$

4. Symmetry cards. FORMAT(F11.6,2I2,F11.6,2I2,F11.6,2I2)
Each of these NS cards describes one symmetry transformation j of the atomic coordinates. For non-centrosymmetric structures, NS is the number of equivalent positions. For centrosymmetric structures (with the origin at a center), NS is half the number of equivalent positions, and only one position of each centrosymmetrically related pair is used. The basic position x, y, z must be included in these cards. See the sample problem for an example of this input.

Columns	
1-11	Translational part of x_j or blank.
12-13	1, 2, 3, -1, -2, -3, or blank for x, y, z, -x, -y, -z, or blank, respectively, as used in the expression for the transformed x_j.
14-15	1, 2, 3, -1, -2, -3, or blank for x, y, z, -x, -y, -z, or blank, respectively, as used in the expression for the transformed x_j. (Columns 12 and 13 are exactly equivalent to 14 and 15. Also, note that an expression such as $x_j = 2x$ must be treated as $x_j = x + x$.)
16-26	Translational part of y_j or blank.
27-30	Integers representing plus or minus x, y, or z in the expression for the transformed y_j as described above.
31-41	Translational part of z_j or blank.
42-45	Integers representing plus or minus x, y, or z in the expression for the transformed z_j.

5. Reciprocal cell data card. FORMAT(6F9.6)

Columns	
1-9	a* in reciprocal Angstroms
10-18	b* in reciprocal Angstroms
19-27	c* in reciprocal Angstroms
28-36	$\cos\alpha^*$
37-45	$\cos\beta^*$
46-54	$\cos\gamma^*$

6. Trial parameter cards.
These cards are included only if IP = 0. Otherwise the trial parameters (in exactly the same format) will be read from the magnetic tape output of cycle IP of a previous job.

A. Scale factor cards. FORMAT(8F9.6)

Columns	
1-9	First scale factor, s_1.
10-18	Second scale factor, s_2.
.	.
.	.
.	.
64-72	Eighth scale factor, s_8.

The scale factors are continued on additional cards if there are more than eight of them.

B. Over-all temperature factor card. FORMAT(F9.6)

Columns	
1-9	T_o, the coefficient for the over-all temperature factor $\exp(-T_o \sin^2\theta/\lambda^2)$.

C. Atom parameter cards.

Two cards are needed for each atom i in the asymmetric unit, where i = 1,2,..., NA.

First card FORMAT(A6,3X,5F9.6)

Columns	
1-6	Any 6 Hollerith characters identifying atom i. These will be printed with the parameter output.
7-9	Blank
10-18	X-ray scattering factor identifier or neutron scattering factor. For x-ray problems (NF $\neq$ 0) this is an integer from one to NF which identifies the scattering factor table to be used for atom i. The scattering factor tables are numbered in the order in which they were read. Include a decimal point after this number. For neutron problems (NF = 0) this is the neutron scattering factor itself.

Columns	
19-27	A multiplier, a_i, applied to the scattering factor of atom i. This number will usually be 1.0 unless symmetry considerations dictate otherwise.
28-36	The coordinate x_i for atom i.
37-45	The coordinate y_i for atom i.
46-54	The coordinate z_i for atom i.

Second card FORMAT(6F9.6)

For isotropic temperature factors (or for isotropic temperature factors converted to anisotropic form before refining):

Columns	
1-9	T_i, the coefficient for the isotropic temperature factor for atom i, $\exp(-T_i \sin^2\theta/\lambda^2)$.

For anisotropic temperature factors:

Columns	
1-9	β_{11i}, a coefficient in the expression for the anisotropic temperature factor for atom i, $\exp[-(\beta_{11i}h^2 + \beta_{22i}k^2 + \beta_{33i}\ell^2 + 2\beta_{12i}hk + 2\beta_{13i}h\ell + 2\beta_{23}k\ell)]$.
10-18	β_{22i}
19-27	β_{33i}
28-36	β_{12i}
37-45	β_{13i}
46-54	β_{23i}

7. Reflection data cards. FORMAT(I1,F8.0,5F9.0)
One card is needed for each reflection observed or for each structure factor to be computed.
$1 \leqslant NO \leqslant 2499$.*

Columns	
1	Blank
2-9	The index h. No decimal point is needed.
10-18	The index k. No decimal point is needed.

Columns	
19-27	The index ℓ. No decimal point is needed.
28-36	The observed value of $\|F\|$ or F^2, whichever is being refined. For structure factor calculations this field may be left blank.
37-45	The standard error of this observation. If IW = 1 on the control card, this field is irrelevant.
46-54	q, where $1 \leqslant q \leqslant NQ$ and s_q is the scale factor to be used in computing this reflection. No decimal point is needed.

8. Observation termination card. FORMAT(I1)

Column	
1	1 as a sentinel for the end of the observation deck.

9. Parameter selection cards. FORMAT(72I1)
These cards specify the NV parameters to be varied. Consider the trial parameters to be stored in the array P in the following order: the NQ scale factors, the over-all temperature factor coefficient, the six or eleven parameters for the first atom, those for the second atom, etc. The parameters for each atom are the scattering factor, the multiplier, the three coordinates, and the one or six temperature factor coefficients. Each column of the parameter selection card contains an integer KI(I) so that if KI(I) = 0, then P(I) will be held constant. If KI(I) = 1, then P(I) will be adjusted.

Six temperature factor coefficients per atom should be assumed if anisotropic temperature factors are specified or if isotropic temperature factors are to be converted to anisotropic form before refining. For isotropic refinements there is only one temperature factor per atom.

Note that for both x-ray and neutron problems the scattering factor is considered to be a parameter. The neutron scattering factor may be adjusted by least squares, but varying an x-ray scattering factor must not be attempted.

First card

Column	
1	KI(1)
2	KI(2)
.	.
.	.
.	.
72	KI(72)

Second card Column	
1	KI(73)
.	.
.	.
.	.
	KI(NP)

TAPES REQUIRED

Listed here are the monitor tape control cards required for operation at the Oak Ridge Central Data Processing Facility. At other installations the necessary tapes should be specified appropriately.

*TAPE(3, POOL, SAVE)

This is required only if IXFE = 1, indicating that data for the Function and Error Program, OR FFE, are to be saved on tape after the final cycle of refinement. This tape is initially rewound and an end-of-file is written upon completion of the job.

*TAPE(4, Reel number, SAVE)

This is required only if IP > 0, indicating that the initial values of the trial parameters are to be taken from this tape, which was written on a previous job.

*TAPE(5, POOL, SAVE)

This is required only if IT = 1, indicating that the adjusted parameters are to be written on this tape after each cycle. This tape is initially rewound and an end-of-file is written upon completion of the job.

*TAPE(6,AUXOUT)

This is required only if IT = 2, indicating that the adjusted parameters are to be written on this tape

*TAPE(6,AUXOUT) Continued

after each cycle. Cards suitable for input to another job will then be punched off-line. This tape is not rewound and no end-of-file is written on it by the program.

*TAPE(9, OUTPUT)

This is the monitor output tape to be listed.

*TAPE(10, INPUT)

This is the monitor input tape prepared from cards.

CARD DECKS PROVIDED

Subprogram	Type	Symbolic card numbers	Column binary card numbers
Calling program	Fortran	1 - 474	1472 - 1560*,†
PRELIM	Fortran	475 - 629	1561 - 1590*
CALC	Fortran	630 - 929	1591 - 1636*
TEST	Fortran	930 - 1018	1637 - 1649*
PTOSB	Fortran	1019 - 1058	1650 - 1658
SBTOP	Fortran	1059 - 1098	1659 - 1667
SMI	FAP	1099 - 1351	1668 - 1681
PATCH (dummy)	Fortran	1352 - 1358	1682 - 1683
RESETX (dummy)	Fortran	1359 - 1365	1684 - 1685
RESETB (dummy)	Fortran	1366 - 1372	1686 - 1687

*The column binary cards provided were compiled and assembled on an IBM 7090. The calling program, PRELIM, CALC, and TEST should be recompiled if they are to be used on an IBM 704, but the remaining subprograms should work satisfactorily on either machine.

†Card No. 1472 is a control card for the Oak Ridge Monitor System. It may not be appropriate at other installations.

Subprogram	Type	Symbolic card numbers	Column binary card numbers
Library routines SQRT, SIN, COS, EXP, and EXIT (which terminates the job) should be inserted here if they are not supplied by the monitor system.			
PATCH (example)	Fortran	1373 - 1389	1688 - 1692
RESETX (example)	Fortran	1390 - 1398	1693 - 1695
RESETB (example)	Fortran	1399 - 1408	1696 - 1698
Transfer card		1409	
Permanent data cards		1410 - 1412†	
Data for example		1413 - 1471	

†These cards must be present on all problems.

GLOSSARY OF SYMBOLS

Arrays are represented by symbols followed by their minimum allowable dimensions. All other symbols refer to single storage variables. Those marked with an asterisk (*) are read as input data.

A	Real component of the structure factor.
*AI(NA)	Atom multipliers, a_i.
AM((NV*(NV+3))/2)	Matrix of the normal equations. This area is also used for the inverse matrix. Only (NV*(NV+1))/2 words are used for the matrix, but NV more are used by the inverter. Only the upper right triangle of the matrix is stored, and this is stored forward in the memory - i.e., backward in the Fortran indexing system. If a_{ij} represents a matrix element, then a_{11} is at AM((NV*(NV+1))/2), a_{12} is at AM((NV*(NV+1))/2-1), etc., a_{22} is at AM((NV*(NV+1))/2-NV), and $a_{NV,NV}$ is at AM(1). For example, if NV = 4, the storage is as illustrated:

a_{11} = AM(10)	a_{12} = AM(9)	a_{13} = AM(8)	a_{14} = AM(7)
	a_{22} = AM(6)	a_{23} = AM(5)	a_{24} = AM(4)
		a_{33} = AM(3)	a_{34} = AM(2)
			a_{44} = AM(1)

*ATOM(NA)	Alphanumeric name of each atom read in with the parameters of that atom and used in the output as a heading for those parameters.
B	Imaginary component of the structure factor.
*BETA(6,NA)	Anisotropic temperature factor coefficients β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23} (in that order) for the NA atoms. If isotropic temperature factors are used, then BETA(1,I) is the coefficient for atom I.
CA	Coefficient of $\partial A/\partial p$ in the expression for $\partial(s_q F)/\partial p$ or $\partial(s_q{}^2F^2)/\partial p$.
CB	Coefficient of $\partial B/\partial p$ in the expression for $\partial(s_q F)/\partial p$ or $\partial(s_q{}^2F^2)\partial p$.
COSIJ	Trigonometric contribution of atom I in symmetry position J. Also used for COSIJ*EXPIJ.
DADAI(NA)	$\partial A/\partial a_i$ - This array is also used for $\sum_j f_i \cos_{ij} \exp_{ij}$.
DADB(6,NA)	$\partial A/\partial \beta_{11i}$, etc. - This array is also used for $\sum_j h_j{}^2 \cos_{ij} \exp_{ij}$, etc.
DADFI(NA)	$\partial A/\partial f_i$ - This array is also used for $\sum_j \cos_{ij} \exp_{ij}$.

DADX(3,NA)	$\partial A/\partial x_i$, $\partial A/\partial y_i$, and $\partial A/\partial z_i$ - This array is also used for $\sum_j h_j \sin_{ij} \exp_{ij}$, etc.
DBDAI(NA)	$\partial B/\partial a_i$ - This array is also used for $\sum_j f_i \sin_{ij} \exp_{ij}$.
DBDB(6,NA)	$\partial B/\partial \beta_{11i}$, etc. - This array is also used for $\sum_j h_j^2 \sin_{ij} \exp_{ij}$, etc.
DBDFI(NA)	$\partial B/\partial f_i$ - This array is also used for $\sum_j \sin_{ij} \exp_{ij}$.
DBDX(3,NA)	$\partial B/\partial x_i$, $\partial B/\partial y_i$, and $\partial B/\partial z_i$ - This array is also used for $\sum_j h_j \cos_{ij} \exp_{ij}$, etc.
DC(NP)	Calculated derivatives of YC with respect to all parameters p.
DFDAI(NA)	$\partial(s_q F)/\partial a_i$ or $\partial(s_q^2 F^2)/\partial a_i$ - Later copied to array DC.
DFDB(6,NA)	$\partial(s_q F)/\partial \beta_{11i}$, etc., or $\partial(s_q^2 F^2)/\partial \beta_{11i}$, etc. Later copied to DC. When isotropic temperature factors are specified, DFDB(1,I) is used for $\partial(s_q F)/\partial T_i$ or $\partial(s_q^2 F^2)/\partial T_i$.
DFDFI(NA)	$\partial(s_q F)/\partial f_i$ or $\partial(s_q^2 F^2)/\partial f_i$. Later copied to array DC.
DFDS(NQ)	$\partial(s_q F)/\partial s_q$ or $\partial(s_q^2 F^2)/\partial s_q$. Later copied to array DC.
DFDTO	$\partial(s_q F)/\partial T_o$ or $\partial(s_q^2 F^2)/\partial T_o$.
DFDX(3,NA)	$\partial(s_q F)/\partial x_i$, etc., or $\partial(s_q^2 F^2)/\partial x_i$, etc. Later copied to DC.
DIAG(NV)	Diagonal elements of the inverse matrix. These are used for calculating the standard errors of the parameters which were varied.
DV(NV)	Derivatives of those parameters which are to be varied, multiplied by the square root of the weight.

DY	YO(I)-YC.
EXPIJ	Anisotropic temperature factor for atom I in symmetry position J.
F	$s_q F$ or $s_q{}^2 F^2$. F is then copied to YC.
FI	Atomic scattering factor, f_i. Also used for $f_i \exp(-T_i \rho)$ and for $-f_i \exp(-T_i \rho)$.
FRACPT	Fractional part of PT.
FTA	$a_i f_i$ for anisotropic temperature factors, or $a_i f_i \exp(-T_i \rho)$ for isotropic temperature factors.
FTACOS	$a_i f_i \exp(-T_i \rho) \sum_j \cos_{ij}$.
FTASIN	$a_i f_i \exp(-T_i \rho) \sum_j \sin_{ij}$.
*FX(32,NF)	Scattering factor tables.
*H(4)	Untransformed indices h, k, and ℓ, and the scale factor specification, q. H is the same as column I or array X.
HHB	Exponential argument.
HHJ(6)	Transformed index products $(h^2)_j$, $(k^2)_j$, $(\ell^2)_j$, $(2hk)_j$, $(2h\ell)_j$, and $(2k\ell)_j$ in that order.
HJ(3)	Transformed indices h_j, k_j, and ℓ_j.
HOLD	Temporary location used in reversing the order of elements of matrix AM.
HX	Trigonometric argument, $h_j x_i + k_j y_i + \ell_j z_i + t_j$.
IC	Identifying number of a particular cycle in the job.
*ICENT	Symmetry indicator. ICENT = 1 for centro-symmetric structures. ICENT = 2 for non-centro-symmetric structures.
*IFSQ	F^2 indicator. If IFSQ = 1 the refinement is based on the scaled structure factors. If IFSQ = 2 the squares of these quantities are used.

IHKL(4)	The array X(4,NO) converted to fixed point numbers for output purposes.
II	Index used so that AM(II) is diagonal element a_{ii}.
IID	Increment subtracted from II to step down diagonal of matrix AM(II).
IJ	Index used so that AM(IJ) is a_{ij}.
IJD	Increment subtracted from IJ to step down a column of matrix AM(IJ).
*IP	Parameter input indicator. If IP = 0 the trial parameters p are to be read as input data. If IP > 0, the parameters are to be taken from the magnetic tape output of cycle IP of a previous job.
IPT	Integral part of PT.
IQ	Independent variable, q, specifying the scale factor, s_q, associated with a given reflection.
*ISENT	Sentinel set at 1 to end the observation deck.
ISING	Singularity indicator set at 1 if a zero diagonal element is found in the original matrix or if a diagonal element becomes zero or negative during inversion by SMI. Otherwise ISING = 0.
*IS(2,3,NS)	Integers representing the non-translational part of the symmetry information. For example, if the Jth symmetry transformation is y-x, -x, 1/3 + z, this information would be stored as follows:

```
TS(1,J)   = 0.0
IS(1,1,J) = 2 (for y)
IS(2,1,J) = -1 (for -x)
TS(2,J)   = 0.0
IS(1,2,J) = -1 (for -x)
IS(2,2,J) = 0
TS(3,J)   = 0.333333
IS(1,3,J) = 3 (for z)
IS(2,3,J) = 0
```

ISTOP	Stop indicator set at 1 by subroutine TEST to indicate that no further cycles are to be run on this job. Otherwise ISTOP = 0.

*IT	Parameter output indicator. If IT = 0, parameters are not to be written on tape for use as input to later least-squares cycles. If IT = 1, they are to be written on a private tape. If IT = 2, they are written on the monitor auxiliary tape in such a way as to yield punched cards. The private tape is initially rewound and is terminated by an end-of-file while the auxiliary tape is not.
*ITF	Temperature factor indicator. ITF = 1 for isotropic temperature factors. ITF = 2 for anisotropic temperature factors. If ITF = 3, the program converts isotropic temperature factor coefficients to anisotropic form before refining.
*IW	Unit weight indicator. If IW = 1, all observations are assigned unit weights. If IW = 0, then the weights are taken as 1.0/SIGYO(I)**2.
*IXFE	Function and error output indicator. If IXFE = 1, information including the parameters and the variance-covariance matrix will be written on a private tape for use by OR FFE. If IXFE = 0, no such output will be made.
JK	Index used so that AM(JK) is a_{jk}.
*KI(NP)	Parameter selection integers. KI(I) = 1 if P(I) is to be varied. Otherwise KI(I) = 0.
*LABEL(2,14)	Alphanumeric labels read in at the start of the problem and used to label each parameter at the time of the output of the old and new parameters.
*NA	Number of atoms in the asymmetric unit.
*NC	Number of cycles of refinement to be performed in the job. The program puts out YC, the calculated values of the scaled structure factor or its square, NC + 1 times. If NC = 0, YC is calculated and put out, but no refinement occurs.
NCY	NC + 1, the number of cycles plus one. This is the number of times the list of YC will be put out.
*NF	Number of different x-ray form factor tables to be used. For neutron diffraction NF = 0.

NM	(NV*(NV + 1))/2, the number of elements in the matrix AM.
NO	Number of observations.
NP	Total number of parameters including those to be varied as well as those to be held constant.
NPCD	Smallest multiple of 8 greater than or equal to NQ. Used for punching scale factors 8 to a card.
*NQ	Number of scale factors in the parameter list.
*NS	Number of symmetry cards. For non-centro-symmetric structures, NS is equal to the number of equivalent positions. For centro-symmetric structures, NS is half the number of equivalent positions.
NT	Number of private or auxiliary tape used for output of parameters to be saved.
*NV	Number of parameters to be varied. If NC = 0, then NV is irrelevant.
NX	Number of independent variables associated with each observation. NX is fixed at 4 in this program.
PDI	PD(I).
PD(NV)	Calculated parameter changes for those parameters which were varied.
PIFI	$-2\pi a_i f_i \exp(-T_i \rho)$ or $2\pi a_i f_i \exp(-T_i \rho)$.
P(NP)	List of NP parameters, some of which will be varied. These are copied from various arrays by the subroutine SBTOP, adjusted, and then restored to the arrays by subroutine PTOSB.
POLD	Parameter before correction is added.
PRCP(6)	Products of the reciprocal cell parameters, $a^{*2}/4$, $b^{*2}/4$, $c^{*2}/4$, $a^*b^*\cos\gamma^*/4$, $a^*c^*\cos\beta^*/4$, $b^*c^*\cos\alpha^*/4$, in that order.
PT	$1.0 + (\sin\theta/\lambda)/.05$. The location of FI in the scattering factor table, FX.
R	R factor in which the summations are made over all non-zero observations.

*RCP(6)	Reciprocal cell parameters, a*, b*, c*, cosα*, cosβ*, cosγ*, in that order.
RHO	$\rho = (\sin\theta/\lambda)^2$ for each reflection.
RNUM	Numerator of R.
ROW(NV)	A row of the correlation matrix ready for output.
RZ	R factor in which the summations are made over all observations, including zero observations.
RZDEN	Denominator of both R and RZ.
RZNUM	Numerator of RZ.
*SC(NQ)	NQ scale factors.
*SF(NA)	For neutron problems, SF(I) is the scattering factor f_i for atom I. For x-ray problems, it is an integer (in floating point form) which defines the scattering factor table to be used.
SIG	(SQRTW*(YO(I)-YC))**2 summed over all observations.
SIGP	Standard error of a parameter.
*SIGYO(NO)	Standard errors of the NO observed structure factors or their squares.
SINIJ	Trigonometric contribution of atom I in position J. Also used for SINIJ*EXPIJ.
SINTHL	$\sin\theta/\lambda = \rho^{1/2}$.
SQRTAB	$(A^2 + B^2)^{1/2}$.
SQRTW	Square root of the weight for each observation.
SQSIG(2)	SQSIG(1) is the error of fit, SQRTF(SIG/FLOATF(NO-NV)). SQSIG(2) is SQSIG(1) saved from the previous cycle of this job. SQSIG(2) will be set to zero for the first cycle of each job.
SQTO	$s_q \exp(-T_o\rho)$ or $s_q^2 \exp(-2T_o\rho)$.
TFI	Isotropic temperature factor, $\exp(-T_i\rho)$.
*TITLE(12)	Alphanumeric title read at start of problem and transcribed to the output.

TJ	Translational term, t_j, for the trigonometric argument, HX.
*TO	Over-all temperature factor coefficient, T_o.
*TS(3,NS)	Translational part of symmetry information. (See IS for an example.)
VARI	SQSIG(1)**2, the constant used to convert the inverse matrix to the variance-covariance matrix.
V(NV)	Vector of the normal equations.
WDY	(YO(I)-YC)/SIGYO(I).
WR	Weighted R factor in which the summations are made over all non-zero observations.
WRNUM	Numerator of WR.
WRZ	Weighted R factor in which the summations are made over all observations, including zero observations.
WRZDEN	Denominator of both WR and WRZ.
WRZNUM	Numerator of WRZ.
*X(4,NO)	Four independent variables for each of NO observations. These are the indices h, k, and ℓ and q, the number specifying the scale factor. The latter will be moved to IQ.
*XYZ(3,NA)	Atomic coordinates x, y, and z for the NA atoms.
YC	Calculated value of the scaled structure factor or its square stored by subroutine CALC.
*YO(NO)	NO observed structure factors or their squares.

SYMBOLIC PROGRAM LISTING

```
*TYPE(FORTRAN)                                                          FLS    1
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS    2
C     CALLING PROGRAM, A MODIFICATION OF OR GLS                         FLS    3
      COMMON NC,NV,NX,IW,IP,IT,NP,ISENT,NO,NM,NCY,IC,SIG,YC             FLS    4
      COMMON SQREW,DY,WDY,JK,ISING,II,IID,PDI,IJ,IJD,POLD               FLS    5
      COMMON SIGP,ISTOP,NT,NPCD,IXFE,HOLD,VARI                          FLS    6
      COMMON TITLE,P,X,YO,SIGYO,KI,SQSIG,AM,V,DC,DV,DIAG,PD,ROW         FLS    7
      COMMON RNUM,RZNUM,RZDEN,WRNUM,WRZNUM,WRZDEN,R,RZ,WR,WRZ           FLS    8
      COMMON LABEL,ATOM,IHKL                                            FLS    9
      COMMON IFSQ,ITF,NF,NA,ICENT,NS,NQ,TO,TJ,HX,HHB,EXPIJ,COSIJ,SINIJ  FLS   10
      COMMON FI,A,B,RHO,SINFHL,PT,IPT,FRACPT,FTA,FTACOS,FTASIN,TFI,PIFI FLS   11
      COMMON IC,SQTO,SQRTAB,F,DFDTO                                     FLS   12
      COMMON SC,SF,AI,XYZ,BETA,DADFI,DBDFI,DADAI,DBDAI,DADX,DBDX,DADB   FLS   13
      COMMON DBDB,DFDS,DFDFI,DFDAI,DFDX,DFDB,TS,IS,HJ,HHJ,RCP,FX,PRCP   FLS   14
      COMMON CA,CB                                                      FLS   15
                                                                        FLS   16
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#230,NO(MAX)#2500,NX(MAX)#4,    FLS   17
C        NF(MAX)#10,NA(MAX)#20,NS(MAX)#24,NQ(MAX)#9                     FLS   18
      DIMENSION TITLE(12),P(230),X(4,2500),YO(2500),SIGYO(2500),KI(230) FLS   19
      DIMENSION SQSIG(2),AM(5150),V(100),DC(230),DV(100)                FLS   20
      DIMENSION DIAG(100),PD(100),ROW(100),ATOM(20),LABEL(2,14),IHKL(4) FLS   21
      DIMENSION SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20),DADFI(20)     FLS   22
      DIMENSION DBDFI(20),DADAI(20),DBDAI(20),DADX(3,20),DBDX(3,20)     FLS   23
      DIMENSION DADB(6,20),DBDB(6,20),DFDS( 9),DFDFI(20),DFDAI(20)      FLS   24
      DIMENSION DFDX(3,20),DFDB(6,20),TS(3,24),IS(2,3,24),HJ(3),H(4)    FLS   25
      DIMENSION HHJ(6),RCP(6),FX(32,10),PRCP(6)                         FLS   26
                                                                        FLS   27
C     FORMAT STATEMENTS                                                 FLS   28
00031 FORMAT(8F9.6,12X)                                                 FLS   29
00032 FORMAT(F9.6,75X)                                                  FLS   30
00033 FORMAT(A6,3X,5F9.6,30X)                                           FLS   31
00034 FORMAT(6F9.6,30X)                                                 FLS   32
00035 FORMAT(69H0INPUT DATA FOR OR-FORTRAN FUNCTION AND ERROR PROGRAM NOFLS   33
     1T TO BE SAVED)                                                    FLS   34
00037 FORMAT(53H0INPUT DATA FOR OR-FORTRAN FUNCTION AND ERROR PROGRAM/  FLS   35
     130H TO BE WRITTEN ON PRIVATE TAPE)                                FLS   36
00041 FORMAT(1H041X,29HNUMERATOR   DENOMINATOR     R)                   FLS   37
00042 FORMAT(25H0R FACTOR INCLUDING ZEROS,17X,F9.3,4X,F9.3,4X,F5.3)     FLS   38
00043 FORMAT(24H0R FACTOR OMITTING ZEROS,18X,F9.3,4X,F9.3,4X,F5.3)      FLS   39
00044 FORMAT(34H0WEIGHTED R FACTOR INCLUDING ZEROS,                     FLS   40
     18X,F9.3,4X,F9.3,4X,F5.3)                                          FLS   41
00046 FORMAT(33H0WEIGHTED R FACTOR OMITTING ZEROS,                      FLS   42
     19X,F9.3,4X,F9.3,4X,F5.3)                                          FLS   43
00051 FORMAT(12A6)                                                      FLS   44
00052 FORMAT(1H112A6)                                                   FLS   45
00053 FORMAT(24I3)                                                      FLS   46
00054 FORMAT(32H0NUMBER OF CYCLES IN THIS JOB ISI2/37H0NUMBER OF PARAMETFLS   47
     1ERS TO BE VARIED ISI4)                                            FLS   48
00061 FORMAT(31H0WEIGHTS TO BE SUPPLIED BY USER)                        FLS   49
00062 FORMAT(34H0UNIT WEIGHTS TO BE SET BY PROGRAM)                     FLS   50
00063 FORMAT(36H0PARAMETERS TO BE READ AS INPUT DATA)                   FLS   51
00064 FORMAT(34H0PARAMETERS TO BE TAKEN FROM CYCLEI2,16H OF PREVIOUS JOBFLS   52
     1)                                                                 FLS   53
00067 FORMAT(29H0NUMBER OF PARAMETERS READ ISI4)                        FLS   54
00068 FORMAT (I1,F8.0,7F9.0)                                            FLS   55
00069 FORMAT(31H0NUMBER OF OBSERVATIONS READ ISI5)                      FLS   56
00070 FORMAT(72I1)                                                      FLS   57
00071 FORMAT(10F12.8)                                                   FLS   58
00072 FORMAT(46H0CALCULATED Y BASED ON PARAMETERS BEFORE CYCLEI2)       FLS   59
00073 FORMAT(97H0   H   K   L    Y(OBS)    Y(CALC)        A          B  FLS   60
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     1    OBS-CALC    SIG(O)  (O-C)/SIG(O)   (Q/1H )                    FLS   61
00078 FORMAT(1H0A6)                                                      FLS   62
00079 FORMAT(1H 3I4,7F11.4,I7)                                           FLS   63
00080 FORMAT(51H0AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE I2/ FLS   64
     120HOSUM(W*(O-C)**2) IS E11.4/35H0SQRTF(SUM(W*(O-C)**2)/(NO-NV)) ISFLS   65
     2 F10.4)                                                            FLS   66
00081 FORMAT(60H0ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CFLS   67
     1YCLE I2/20HOSUM(W*(O-C)**2) IS E11.4/35H0SQRTF(SUM(W*(O-C)**2)/(NOFLS   68
     2-NV)) IS F10.4)                                                    FLS   69
00083 FORMAT(62H MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PARFLS   70
     1AMETER13,16H OF THOSE VARIED)                                      FLS   71
00085 FORMAT(40H SINGULARITY RETURN FROM MATRIX INVERTER)                FLS   72
00086 FORMAT(37H0PARAMETERS AFTER LEAST SQUARES CYCLE12/64H0 PARAMETER   FLS   73
     1         OLD         CHANGE          NEW          ERROR)          FLS   74
00088 FORMAT(1H02A6,F14.7,13X,F13.7)                                     FLS   75
00089 FORMAT(1H02A6,1X,4F13.7)                                           FLS   76
00090 FORMAT(66H0SUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FLS   77
     1FOR REASON12)                                                      FLS   78
00092 FORMAT(11H0INPUT DATA/20H0  I      P(I)  K1(I)/1H )                FLS   79
00093 FORMAT(1H I3,F10.4,I4)                                             FLS   80
00094 FORMAT(51H0CORRECTED PARAMETERS NOT TO BE SAVED FOR LATER USE)     FLS   81
00095 FORMAT(51H0CORRECTED PARAMETERS TO BE WRITTEN ON PRIVATE TAPE)     FLS   82
00096 FORMAT(51H0CORRECTED PARAMETERS TO BE WRITTEN FOR CARD OUTPUT)     FLS   83
00097 FORMAT(19H0CORRELATION MATRIX)                                     FLS   84
00098 FORMAT(1H0I3,10F9.4/(1H 3X,10F9.4))                                FLS   85
00099 FORMAT(8E15.8)                                                     FLS   86
                                                                         FLS   87
C     READ TITLE AND CONTROL CARD                                        FLS   88
      READ INPUT TAPE 10,00051,((LABEL(L,K),L#1,2),K#1,14)               FLS   89
      READ INPUT TAPE 10,00051,(TITLE(I),I#1,12)                         FLS   90
      WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                        FLS   91
      READ INPUT TAPE 10,00053,NC,NV,IW,IP,IT,IXFE                       FLS   92
      NX#4                                                               FLS   93
      WRITE OUTPUT TAPE 9,00054,NC,NV                                    FLS   94
00207 IF(IW)00210,00208,00210                                            FLS   95
                                                                         FLS   96
00208    WRITE OUTPUT TAPE 9,00061                                       FLS   97
         GO TO 00211                                                     FLS   98
                                                                         FLS   99
00210    WRITE OUTPUT TAPE 9,00062                                       FLS  100
                                                                         FLS  101
00211 IF(IP)00212,00212,00214                                            FLS  102
                                                                         FLS  103
00212    WRITE OUTPUT TAPE 9,00063                                       FLS  104
         GO TO 00215                                                     FLS  105
                                                                         FLS  106
00214    WRITE OUTPUT TAPE 9,00064,IP                                    FLS  107
                                                                         FLS  108
00215 IF(IT-1)00216,00218,00221                                          FLS  109
                                                                         FLS  110
00216    WRITE OUTPUT TAPE 9,00094                                       FLS  111
         GO TO 00222                                                     FLS  112
                                                                         FLS  113
00218    WRITE OUTPUT TAPE 9,00095                                       FLS  114
         REWIND 5                                                        FLS  115
         GO TO 00222                                                     FLS  116
                                                                         FLS  117
00221    WRITE OUTPUT TAPE 9,00096                                       FLS  118
                                                                         FLS  119
00222 IF(IXFE)00225,00223,00225                                          FLS  120
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                                                                        FLS  121
00223     WRITE OUTPUT TAPE 9,C0035                                     FLS  122
          GO TO 00301                                                   FLS  123
                                                                        FLS  124
00225     WRITE OUTPUT TAPE 9,C0037                                     FLS  125
          REWIND 3                                                      FLS  126
                                                                        FLS  127
C       ENTER PRELIM TO READ CRYSTALLOGRAPHIC INPUT                     FLS  128
00301 CALL PRELIM                                                       FLS  129
00601 WRITE OUTPUT TAPE 9,C0067,NP                                      FLS  130
                                                                        FLS  131
C       READ OBSERVATIONS TO SENTINEL                                   FLS  132
        J#0                                                             FLS  133
                                                                        FLS  134
00801     J#J+1                                                         FLS  135
          READ INPUT TAPE IO,C0068,ISENT,(X(I,J),I#1,3),YO(J),SIGYO(J), FLS  136
     1                                                   X(4,J)         FLS  137
          IF(ISENT)00801,00801,01101                                    FLS  138
                                                                        FLS  139
01101 NO#J-1                                                            FLS  140
        WRITE OUTPUT TAPE 9,C0069,NO                                    FLS  141
                                                                        FLS  142
C       READ KEY INTEGERS IF REFINEMENT IS TO BE MADE                   FLS  143
        IF(NO)01601,01601,01301                                         FLS  144
                                                                        FLS  145
01301     READ INPUT TAPE IO,C0070,(KI(I),I#1,NP)                       FLS  146
                                                                        FLS  147
C       INITIALIZE PROBLEM                                              FLS  148
01601 NM#(NV*(NV+1))/2                                                  FLS  149
        SQSIG(1)#0.0                                                    FLS  150
                                                                        FLS  151
C       PUT OUT TRIAL PARAMETERS AND KEY INTEGERS                       FLS  152
        WRITE OUTPUT TAPE 9,C0092                                       FLS  153
        DO 01653 I#1,NP                                                 FLS  154
                                                                        FLS  155
01653     WRITE OUTPUT TAPE 9,C0093,I,P(I),KI(I)                        FLS  156
                                                                        FLS  157
C       START LOOP TO PERFORM NC CYCLES AND ONE FINAL CALCULATION OF Y  FLS  158
        NCY#NC+1                                                        FLS  159
        DO 08501 IC#1,NCY                                               FLS  160
                                                                        FLS  161
C         CLEAR ARRAYS AM AND V EXCEPT ON LAST CYCLE                    FLS  162
          IF(IC-NCY)01851,02001,02001                                   FLS  163
                                                                        FLS  164
01851       DO 01852 I#1,NM                                             FLS  165
                                                                        FLS  166
01852          AM(I)#0.0                                                FLS  167
                                                                        FLS  168
            DO 01902 I#1,NV                                             FLS  169
                                                                        FLS  170
01902          V(I)#0.0                                                 FLS  171
                                                                        FLS  172
C         INITIALIZE FOR CYCLE IC AND PUT OUT CAPTION FOR LIST OF Y(CALC)FLS  173
02001     SQSIG(2)#SQSIG(1)                                             FLS  174
          SIG#0.0                                                       FLS  175
          RNUM#0.0                                                      FLS  176
          RZNUM#0.0                                                     FLS  177
          RZDEN#0.0                                                     FLS  178
          WRNUM#0.0                                                     FLS  179
          WRZNUM#0.0                                                    FLS  180
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      WRZDEN#0.0                                                        FLS  181
      WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                       FLS  182
      WRITE OUTPUT TAPE 9,00072,IC                                      FLS  183
      WRITE OUTPUT TAPE 9,00073                                         FLS  184
                                                                        FLS  185
C     START LOOP THROUGH NO OBSERVATIONS                                FLS  186
02201 DO 05101 I#1,NO                                                   FLS  187
                                                                        FLS  188
C        ENTER SUBROUTINE CALC TO COMPUTE Y(CALC) AND DERIVATIVES       FLS  189
         CALL CALC(X(1,I),YC,P,DC)                                      FLS  190
                                                                        FLS  191
C        OBTAIN WEIGHT AND CALCULATE QUANTITIES FROM Y(OBS)-Y(CALC)     FLS  192
         IF(IW)02601,02501,02601                                        FLS  193
                                                                        FLS  194
02501       SQRTW#1.0/SIGYO(I)                                          FLS  195
            GO TO 02701                                                 FLS  196
                                                                        FLS  197
02601       SIGYO(I)#1.0                                                FLS  198
            SQRTW#1.0                                                   FLS  199
                                                                        FLS  200
02701    DY#YO(I)-YC                                                    FLS  201
         WDY#SQRTW*DY                                                   FLS  202
         SIG#SIG+WDY*WDY                                                FLS  203
         RZNUM#RZNUM+ABSF(DY)                                           FLS  204
         RZDEN#RZDEN+ABSF(YO(I))                                        FLS  205
         WRZNUM#WRZNUM+WDY**2                                           FLS  206
         WRZDEN#WRZDEN+(SQRTW*YO(I))**2                                 FLS  207
         IF(YO(I))02752,02801,02752                                     FLS  208
                                                                        FLS  209
02752       RNUM#RNUM+ABSF(DY)                                          FLS  210
            WRNUM#WRNUM+WDY**2                                          FLS  211
                                                                        FLS  212
C        PUT OUT Y(CALC) AND OTHER INFORMATION FOR ONE OBSERVATION      FLS  213
02801    DO 02802 K#1,4                                                 FLS  214
                                                                        FLS  215
02802       IHKL(K)#X(K,I)                                              FLS  216
                                                                        FLS  217
         WRITE OUTPUT TAPE 9,00079,(IHKL(K),K#1,3),YO(I),YC,A,B,DY,     FLS  218
     1                                   SIGYO(I),WDY,IHKL(4)           FLS  219
                                                                        FLS  220
C        BY-PASS DERIVATIVE AND MATRIX SET-UP ON FINAL CALC OF Y        FLS  221
         IF(IC-NCY)03001,05101,05101                                    FLS  222
                                                                        FLS  223
C           START LOOP TO STORE AN ARRAY OF NV DERIVATIVES              FLS  224
03001       J#1                                                         FLS  225
            DO 04101 K#1,NP                                             FLS  226
                                                                        FLS  227
               IF(KI(K))04101,04101,03301                               FLS  228
                                                                        FLS  229
03301             DV(J)#SQRTW*DC(K)                                     FLS  230
                                                                        FLS  231
04001          J#J+1                                                    FLS  232
04101          CONTINUE                                                 FLS  233
C              END LOOP TO OBTAIN DERIVATIVES                           FLS  234
                                                                        FLS  235
C           START LOOP TO STORE MATRIX AND VECTOR. SEE GLOSSARY FOR     FLS  236
C                                                  STORAGE SCHEME       FLS  237
            JK#NM                                                       FLS  238
            DO 05001 J#1,NV                                             FLS  239
                                                                        FLS  240
```

```
04301          IF(DV(J))04501,04401,04501
C                 BY-PASS IF DERIVATIVE IS ZERO
04401             JK#JK-NV+J-1
                  GO TO 05001
04501             DO 04801 K#J,NV
                     AM(JK)#AM(JK)+DV(J)*DV(K)
                     JK#JK-1
04801                CONTINUE
                  V(J)#V(J)+DV(J)*WDY
05001             CONTINUE
C                 END LOOP TO STORE MATRIX AND VECTOR
05101        CONTINUE
C            END LOOP THROUGH NO OBSERVATIONS
C       COMPUTE AND PUT OUT AGREEMENT FACTORS
        SQSIG(I)#SQRTF(SIG/FLOATF(NO-NV))
        WRITE OUTPUT TAPE 9,00081,IC,SIG,SQSIG(I)
        WRNUM#SQRTF(WRNUM)
        WRZNUM#SQRTF(WRZNUM)
        WRZDEN#SQRTF(WRZDEN)
        R#RNUM/RZDEN
        RZ#RZNUM/RZDEN
        WR#WRNUM/WRZDEN
        WRZ#WRZNUM/WRZDEN
        WRITE OUTPUT TAPE 9,00041
        WRITE OUTPUT TAPE 9,00042,RZNUM,RZDEN,RZ
        WRITE OUTPUT TAPE 9,00043,RNUM,RZDEN,R
        WRITE OUTPUT TAPE 9,00044,WRZNUM,WRZDEN,WRZ
        WRITE OUTPUT TAPE 9,00046,WRNUM,WRZDEN,WR
C       BY-PASS MATRIX INVERSION AND PARAMETER OUTPUT ON FINAL CYCLE
        IF(IC-NCY)05401,08701,08701
C          START LOOP TO TEST FOR ZERO DIAGONAL ELEMENT
05401      ISING#0
           II#NM
           IID#NV
           DO 05801 I#1,NV
              IF(AM(II))05701,05601,05701
05601            ISING#1
                 WRITE OUTPUT TAPE 9,00083,I
05701         II#II-IID
              IID#IID-1
05801         CONTINUE
C             END LOOP TO TEST FOR ZERO DIAGONAL ELEMENT
C          TERMINATE JOB IF ZERO DIAGONAL ELEMENT WAS FOUND
           IF(ISING)11501,06001,11501
C             ENTER SUBROUTINE TO REPLACE MATRIX WITH INVERSE
06001         CALL SMI(AM(NM),NV,ISING)
              IF(ISING)06201,06301,06201
```

```
C                 TERMINATE JOB IF SINGULAR MATRIX WAS FOUND
06201             WRITE OUTPUT TAPE 9,00085
                  GO TO 11501

C                 START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR
C                                                PARAMETER CHANGES
06301             DO 07201 I#1,NV

                     PDI#0.0
                     IJ#NM-I+1
                     IJD#NV-1
                     DO 07001 J#1,NV

                        PDI#PDI+AM(IJ)*V(J)
                        IF(J-1)06701,06801,06901

06701                      IJ#IJ-IJD
                           IJD#IJD-1
                           GO TO 07001

C                          SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX
06801                      DIAG(I)#AM(IJ)

06901                      IJ#IJ-1
07001                      CONTINUE

                     PD(I)#PDI
                     SIG#SIG-PDI*V(I)
07201                CONTINUE
C                    END LOOP FOR MATRIX VECTOR MULTIPLICATION

C                 RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG
                  SQSIG(1)#SQRTF(SIG/FLOATF(ND-NV))

C                 PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS
                  WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)
                  WRITE OUTPUT TAPE 9,00086,IC

C                 START LOOP TO CORRECT AND PUT OUT PARAMETERS
                  J#1
                  N#1
                  DO 08001 I#1,NP

C                    SET K TO SELECT APPROPRIATE LABEL
                     IF(I-NQ-1)07452,07454,07456

07452                   K#1
                        GO TO 07501

07454                   K#2
                        GO TO 07501

07456                   IF(ITF-1)07457,07457,07461

07457                      K#XMODF(I-NQ-2,6)+3
                           IF(K-8)07462,07459,07459

07459                         K#14
                              GO TO 07501
```

```
07461                    K#XMODF(I-NQ-2,11)+3
07462              IF(K-3)07501,07463,07501
07463                 WRITE OUTPUT TAPE 9,00078,ATOM(N)
                      N#N+1
C                  TEST KEY INTEGERS
07501              IF(KI(I))07601,07601,07701
07601                 WRITE OUTPUT TAPE 9,00088,(LABEL(L,K),L#1,2),
     1                                                P(I),P(I)
                      GO TO 08001
07701                 POLD#P(I)
                      P(I)#POLD+PD(J)
                      SIGP#SQRTF(DIAG(J))*SQSIG(1)
                      WRITE OUTPUT TAPE 9,00089,(LABEL(L,K),L#1,2),
     1                                          POLD,PD(J),P(I),SIGP
                      J#J+1
08001              CONTINUE
C                  END LOOP TO CORRECT AND PUT OUT PARAMETERS
C               PUT OUT ESTIMATED AGREEMENT FACTORS
                WRITE OUTPUT TAPE 9,00081,IC,SIG,SQSIG(1)
C               ENTER SUBROUTINE TO TEST PARAMETERS
                ISTOP#0
                CALL TEST
C               WRITE CORRECTED PARAMETERS ON AUXILIARY TAPE IF
C                                                  DESIRED
08201           IF(IT)08202,08301,08202
08202              NT#IT+4
                   NPCD#8*((NQ-1)/8+1)
                   WRITE OUTPUT TAPE NT,00031,(SC(I),I#1,NPCD)
                   WRITE OUTPUT TAPE NT,00032,TO
                   DO 08209 I#1,NA
                      WRITE OUTPUT TAPE NT,00033,ATOM(I),SF(I),AI(I),
     1                                          (XYZ(K,I),K#1,3)
08209                 WRITE OUTPUT TAPE NT,00034,(BETA(K,I),K#1,6)
C               TERMINATE JOB IF INDICATED BY USERS SUBROUTINE TEST
08301           IF(ISTOP)08401,08501,08401
08401              WRITE OUTPUT TAPE 9,00090,ISTOP
                   GO TO 08701
08501              CONTINUE
C                  END LOOP THROUGH NC CYCLES AND FINAL CALC OF Y
C     TERMINATE JOB
08701 IF(NC)11701,11701,08801
C        CALCULATE AND PUT OUT CORRELATION MATRIX
08801    WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)
```

```
      WRITE OUTPUT TAPE 9,CC097                                         FLS  421
      DO 0910I I#1,NV                                                   FLS  422
                                                                        FLS  423
         DIAG(I)#1.0/SQRTF(DIAG(I))                                     FLS  424
0910I    CONTINUE                                                       FLS  425
                                                                        FLS  426
      IJ#NM                                                             FLS  427
      DO 1020I I#1,NV                                                   FLS  428
                                                                        FLS  429
         DO 0960I J#I,NV                                                FLS  430
                                                                        FLS  431
            ROW(J)#0.0                                                  FLS  432
0960I       CONTINUE                                                    FLS  433
                                                                        FLS  434
         DO 1000I J#I,NV                                                FLS  435
                                                                        FLS  436
            ROW(J)#AM(IJ)*DIAG(I)*DIAG(J)                               FLS  437
            IJ#IJ-1                                                     FLS  438
1000I       CONTINUE                                                    FLS  439
                                                                        FLS  440
         WRITE OUTPUT TAPE 9,CCC98,I,(ROW(J),J#I,NV)                    FLS  441
1020I    CONTINUE                                                       FLS  442
                                                                        FLS  443
C     WRITE DATA REQUIRED FOR FUNCTION AND ERROR PROGRAM                FLS  444
1050I IF(IXFE)1060I,1150I,1060I                                         FLS  445
                                                                        FLS  446
1060I    WRITE OUTPUT TAPE 3,CC053,ITF,NQ,NP                            FLS  447
      WRITE OUTPUT TAPE 3,C0071,(P(I),I#1,NP)                           FLS  448
      WRITE OUTPUT TAPE 3,C007C,(K1(I),I#1,NP)                          FLS  449
      WRITE OUTPUT TAPE 3,CC053,NV                                      FLS  450
                                                                        FLS  451
      VARI#SQSIG(1)**2                                                  FLS  452
      DO 1070I I#1,NM                                                   FLS  453
                                                                        FLS  454
1070I    AM(I)#AM(I)*VARI                                               FLS  455
                                                                        FLS  456
      K#NM/2                                                            FLS  457
      L#NM                                                              FLS  458
      DO 1120I I#1,K                                                    FLS  459
                                                                        FLS  460
         HOLD#AM(I)                                                     FLS  461
         AM(I)#AM(L)                                                    FLS  462
         AM(L)#HOLD                                                     FLS  463
         L#L-1                                                          FLS  464
1120I    CONTINUE                                                       FLS  465
                                                                        FLS  466
      WRITE OUTPUT TAPE 3,CC099,(AM(I),I#1,NM)                          FLS  467
      END FILE 3                                                        FLS  468
1150I IF(IT-1)1170I,1160I,1170I                                         FLS  469
                                                                        FLS  470
1160I    END FILE 5                                                     FLS  471
                                                                        FLS  472
1170I CALL EXIT                                                         FLS  473
      END                                                               FLS  474


*TYPE(FORTRAN)                                                          FLS  475
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS  476
C     READ CRYSTAL STRUCTURE DATA AND STORE PARAMETERS                  FLS  477
```

```
      SUBROUTINE PRELIM
      COMMON NC,NV,NX,IW,IP,IT,NP,ISENT,NO,NM,NCY,IC,SIG,YC
      COMMON SQRTW,DY,WDY,JK,ISING,II,IID,PDI,IJ,IJD,POLD
      COMMON SIGP,ISTOP,NT,NPCD,IXFE,HOLD,VARI
      COMMON TITLE,P,X,YO,SIGYO,KI,SQSIG,AM,V,DC,DV,DIAG,PD,ROW
      COMMON RNUM,RZNUM,RZDEN,WRNUM,WRZNUM,WRZDEN,R,RZ,WR,WRZ
      COMMON LABEL,ATOM,IHKL
      COMMON IFSQ,ITF,NF,NA,ICENT,NS,NQ,TO,TJ,HX,HHB,EXPIJ,COSIJ,SINIJ
      COMMON FI,A,B,RHO,SINTHL,PT,IPT,FRACPT,FTA,FTACOS,FTASIN,TFI,PIFI
      COMMON IQ,SQTO,SQRTAB,F,DFDTO
      COMMON SC,SF,AI,XYZ,BETA,DADFI,DBDFI,DADAI,DBDAI,DADX,DBDX,DADB
      COMMON DBDB,DFDS,DFDFI,DFDAI,DFDX,DFDB,TS,IS,HJ,HHJ,RCP,FX,PRCP
      COMMON CA,CB
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#230,NO(MAX)#2500,NX(MAX)#4,
C        NF(MAX)#10,NA(MAX)#20,NS(MAX)#24,NQ(MAX)#9
      DIMENSION TITLE(12),P(230),X(4,2500),YO(2500),SIGYO(2500),KI(230)
      DIMENSION SQSIG(2),AM(5150),V(100),DC(230),DV(100)
      DIMENSION DIAG(100),PD(100),ROW(100),ATOM(20),LABEL(2,14),IHKL(4)
      DIMENSION SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20),DADFI(20)
      DIMENSION DBDFI(20),DADAI(20),DBDAI(20),DADX(3,20),DBDX(3,20)
      DIMENSION DADB(6,20),DBDB(6,20),DFDS( 9),DFDFI(20),DFDAI(20)
      DIMENSION DFDX(3,20),DFDB(6,20),TS(3,24),IS(2,3,24),HJ(3),H(4)
      DIMENSION HHJ(6),RCP(6),FX(32,10),PRCP(6)
C     READ AND PUT OUT CONTROL INFORMATION
      READ INPUT TAPE 10,2,IFSQ,ITF,NF,NA,ICENT,NS,NQ
    2 FORMAT (7I3)
      IF(IFSQ-1)4,4,7
    4    WRITE OUTPUT TAPE 9,5
    5    FORMAT (11HOBASED ON F)
         GO TO 9
    7    WRITE OUTPUT TAPE 9,8
    8    FORMAT (19HOBASED ON F SQUARED)
    9 IF(ITF-2)10,13,16
   10    WRITE OUTPUT TAPE 9,11
   11    FORMAT (30HOISOTROPIC TEMPERATURE FACTORS)
         GO TO 19
   13    WRITE OUTPUT TAPE 9,14
   14    FORMAT (32HOANISOTROPIC TEMPERATURE FACTORS)
         GO TO 19
   16    WRITE OUTPUT TAPE 9,17
   17    FORMAT (43HOISOTROPIC TEMPERATURE FACTORS CONVERTED TO,
     1      28H ANISOTROPIC BEFORE REFINING)
   19 WRITE OUTPUT TAPE 9,20,NF
   20 FORMAT (38HONUMBER OF SCATTERING FACTOR TABLES IS I3)
      WRITE OUTPUT TAPE 9,22,NA
   22 FORMAT (38HONUMBER OF ATOMS IN ASYMMETRIC UNIT IS I3)
      IF(ICENT-1)24,24,27
   24    WRITE OUTPUT TAPE 9,25
```

```
   25    FORMAT (16H0CENTROSYMMETRIC)                                    FLS  538
         GO TO 29                                                        FLS  539
                                                                         FLS  540
   27    WRITE OUTPUT TAPE 9,28                                          FLS  541
   28    FORMAT (20H0NON-CENTROSYMMETRIC)                                FLS  542
                                                                         FLS  543
   29 WRITE OUTPUT TAPE 9,30,NS                                          FLS  544
   30 FORMAT (28H0NUMBER OF SYMMETRY CARDS IS I3)                        FLS  545
      WRITE OUTPUT TAPE 9,32,NQ                                          FLS  546
   32 FORMAT (27H0NUMBER OF SCALE FACTORS IS I3)                         FLS  547
                                                                         FLS  548
C     READ AND PUT OUT SCATTERING FACTOR TABLES                          FLS  549
      IF(NF)40,60,40                                                     FLS  550
                                                                         FLS  551
   40    READ INPUT TAPE 10,50,((FX(I,J),I#1,32),J#1,NF)                 FLS  552
   50    FORMAT (8F9.3)                                                  FLS  553
         DO 56 J#1,NF                                                    FLS  554
                                                                         FLS  555
            WRITE OUTPUT TAPE 9,55,J                                     FLS  556
   55       FORMAT (24H0SCATTERING FACTOR TABLEI3/1H )                   FLS  557
   56       WRITE OUTPUT TAPE 9,57,(FX(I,J),I#1,32)                      FLS  558
   57       FORMAT (1H 8F12.3)                                           FLS  559
                                                                         FLS  560
C     READ AND PUT OUT SYMMETRY TRANSFORMATIONS                          FLS  561
   60 READ INPUT TAPE 10,70,((TS(1,J),(IS(K,I,J),K#1,2),I#1,3),J#1,NS)   FLS  562
   70 FORMAT (F11.6,2I2,F11.6,2I2,F11.6,2I2)                             FLS  563
      WRITE OUTPUT TAPE 9,74                                             FLS  564
   74 FORMAT (21H0SYMMETRY INFORMATION/67H0     TRANSFORMED X            FLS  565
     1TRANSFORMED Y            TRANSFORMED Z/1H )                       FLS  566
      WRITE OUTPUT TAPE 9,76,((TS(I,J),(IS(K,I,J),K#1,2),I#1,3),J#1,NS) FLS  567
   76 FORMAT (1H F13.6,2I2,F20.6,2I2,F20.6,2I2)                          FLS  568
                                                                         FLS  569
C     READ AND PUT OUT RECIPROCAL CELL PARAMETERS                        FLS  570
      READ INPUT TAPE 10,90,(RCP(K),K#1,6)                               FLS  571
   90 FORMAT (6F9.6)                                                     FLS  572
      WRITE OUTPUT TAPE 9,94,(RCP(K),K#1,6)                              FLS  573
   94 FORMAT (29H0RECIPROCAL CELL PARAMETERS  6F11.6)                    FLS  574
      PRCP(1)#RCP(1)**2*.25                                              FLS  575
      PRCP(2)#RCP(2)**2*.25                                              FLS  576
      PRCP(3)#RCP(3)**2*.25                                              FLS  577
      PRCP(4)#RCP(1)*RCP(2)*RCP(6)*.25                                   FLS  578
      PRCP(5)#RCP(1)*RCP(3)*RCP(5)*.25                                   FLS  579
      PRCP(6)#RCP(2)*RCP(3)*RCP(4)*.25                                   FLS  580
                                                                         FLS  581
C     SET TAPE NUMBER FOR PARAMETER INPUT                                FLS  582
      IF(IP)130,140,130                                                  FLS  583
                                                                         FLS  584
  130    NT#4                                                            FLS  585
         REWIND 4                                                        FLS  586
         GO TO 150                                                       FLS  587
                                                                         FLS  588
  140    NT#10                                                           FLS  589
         IP#1                                                            FLS  590
                                                                         FLS  591
C     START LOOP TO READ PARAMETERS UNTIL DESIRED SET                    FLS  592
C                                              HAS BEEN READ             FLS  593
  150 DO 190 J#1,IP                                                      FLS  594
                                                                         FLS  595
         READ INPUT TAPE NT,170,(SC(I),I#1,NQ)                           FLS  596
  170    FORMAT (8F9.6)                                                  FLS  597
```

```
      READ INPUT TAPE NT,170,YO                                         FLS  598
      DO 190 I#1,NA                                                     FLS  599
                                                                        FLS  600
         READ INPUT TAPE NT,200,ATOM(I),SF(I),AI(I),(XYZ(K,I),K#1,3)    FLS  601
190      READ INPUT TAPE NT,210,(BETA(K,I),K#1,6)                       FLS  602
200      FORMAT (A6,3X,5F9.6)                                           FLS  603
210      FORMAT (6F9.6)                                                 FLS  604
                                                                        FLS  605
C     CONVERT ISOTROPIC TEMPERATURE FACTOR TO ANISOTROPIC IF SPECIFIED  FLS  606
      IF (ITF-3)280,230,280                                             FLS  607
                                                                        FLS  608
230   DO 260 I#1,NA                                                     FLS  609
                                                                        FLS  610
         TFI#BETA(1,I)                                                  FLS  611
         DO 260 K#1,6                                                   FLS  612
                                                                        FLS  613
260         BETA(K,I)#TFI*PRCP(K)                                       FLS  614
                                                                        FLS  615
270   ITF#2                                                             FLS  616
                                                                        FLS  617
C     COMPUTE THE TOTAL NUMBER OF PARAMETERS                            FLS  618
280 IF(ITF-1)310,290,310                                                FLS  619
                                                                        FLS  620
290   NP#6*NA+NQ+1                                                      FLS  621
      GO TO 320                                                         FLS  622
                                                                        FLS  623
310   NP#11*NA+NQ+1                                                     FLS  624
                                                                        FLS  625
C     COPY PARAMETERS INTO THE ARRAY P                                  FLS  626
320 CALL SBTOP(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)                     FLS  627
      RETURN                                                            FLS  628
      END                                                               FLS  629


*TYPE(FORTRAN)                                                          FLS  630
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS  631
C     CALCULATE STRUCTURE FACTOR AND DERIVATIVES FOR ONE REFLECTION     FLS  632
                                                                        FLS  633
      SUBROUTINE CALC(H,Y,PAR,DER)                                      FLS  634
                                                                        FLS  635
      COMMON NC,NV,NX,IW,IP,II,NP,ISENT,NO,NM,NCY,IC,SIG,YC             FLS  636
      COMMON SQRTW,DY,WDY,JK,ISING,II,IID,PDI,IJ,IJD,POLD               FLS  637
      COMMON SIGP,ISTOP,NT,NPCD,IXFE,HOLD,VARI                          FLS  638
      COMMON TITLE,P,X,YO,SIGYO,KI,SQSIG,AM,V,DC,DV,DIAG,PD,ROW         FLS  639
      COMMON RNUM,RZNUM,RZDEN,WRNUM,WRZNUM,WRZDEN,R,RZ,WR,WRZ           FLS  640
      COMMON LABEL,ATOM,IHKL                                            FLS  641
      COMMON IFSQ,ITF,NF,NA,ICENT,NS,NQ,TO,TJ,HX,HHB,EXPIJ,COSIJ,SINIJ  FLS  642
      COMMON FI,A,B,RHO,SINTHL,PY,IPT,FRACPT,FTA,FTACOS,FTASIN,TFI,PIFI FLS  643
      COMMON IQ,SQTO,SQRTAB,F,DFDTO                                     FLS  644
      COMMON SC,SF,AI,XYZ,BETA,DADFI,DBDFI,DADAI,DBDAI,DADX,DBDX,DADB   FLS  645
      COMMON DBDB,DFDS,DFDFI,DFDAI,DFDX,DFDB,TS,IS,HJ,HHJ,RCP,FX,PRCP   FLS  646
      COMMON CA,CB                                                      FLS  647
                                                                        FLS  648
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#230,NO(MAX)#2500,NX(MAX)#4,    FLS  649
C        NF(MAX)#10,NA(MAX)#20,NS(MAX)#24,NQ(MAX)#9                     FLS  650
      DIMENSION TITLE(12),P(230),X(4,2500),YO(2500),SIGYO(2500),KI(230) FLS  651
      DIMENSION SQSIG(2),AM(150),V(100),DC(230),DV(100)                 FLS  652
      DIMENSION DIAG(100),PD(100),ROW(100),ATOM(20),LABEL(2,14),IHKL(4) FLS  653
      DIMENSION SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20),DADFI(20)     FLS  654
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```
      DIMENSION DBDFI(20),DADAI(20),DBDAI(20),DADX(3,20),DBDX(3,20)
      DIMENSION DADB(6,20),DBDB(6,20),DFDS( 9),DFDFI(20),DFDAI(20)
      DIMENSION DFDX(3,20),DFDB(6,20),TS(3,24),IS(2,3,24),HJ(3),H(4)
      DIMENSION HHJ(6),RCP(6),FX(32,10),PRCP(6)

C     COMPUTE REQUIRED SUMS OVER NS SYMMETRY TRANSFORMATIONS
C                                          FOR EACH OF NA ATOMS
C     CLEAR STORAGE ARRAYS
      DO 109 I#1,NA

         DADFI(I)#0.0
         DBDFI(I)#0.0
         DO 106 K#1,3

            DADX(K,I)#0.0
 106        DBDX(K,I)#0.0

         DO 109 K#1,6

            DADB(K,I)#0.0
 109        DBDB(K,I)#0.0

C     START LOOP THROUGH THE NS SYMMETRY TRANSFORMATIONS
      DO 2301 J#1,NS

C        STORE TRANSFORMED INDICES
         TJ#0.0
         DO 316 I#1,3

            TJ#TJ+H(I)*TS(I,J)
            HJ(I)#0.0
            DO 315 K#1,3

               KKK#K
               DO 314 L#1,2

                  LLL#L
                  M#IS(L,K,J)
                  IF(M-I)312,311,312

 311                 HJ(I)#HJ(I)+H(K)
                     GO TO 314

 312              IF(M+I)314,313,314

 313                 HJ(I)#HJ(I)-H(K)

 314              CONTINUE

 315           CONTINUE

 316        CONTINUE

C        COMPUTE PRODUCTS OF TRANSFORMED INDICES
         HHJ(1)#HJ(1)**2
         HHJ(2)#HJ(2)**2
         HHJ(3)#HJ(3)**2
         HHJ(4)#2.0*HJ(1)*HJ(2)
         HHJ(5)#2.0*HJ(1)*HJ(3)
         HHJ(6)#2.0*HJ(2)*HJ(3)
```

```
C         START LOOP THROUGH THE NA ATOMS
          DO 2201 I#1,NA

C            ENTER USERS SUBROUTINE TO SET INDICES FOR SPECIAL POSITIONS
             CALL PATCH(I,TJ,HJ,HHJ)

C            COMPUTE TRIGONOMETRIC TERMS
             HX#TJ
             DO 603 K#1,3

  603           HX#HX+HJ(K)*XYZ(K,I)

             COSIJ#COSF(6.28318531*HX)
             SINIJ#SINF(6.28318531*HX)

C            COMPUTE ANISOTROPIC TEMPERATURE FACTOR
             IF(ITF-1)901,901,801

  801           HHB#0.0
                DO 803 K#1,6

  803              HHB#HHB+HHJ(K)*BETA(K,I)

                EXPIJ#EXPF(-HHB)
                COSIJ#COSIJ*EXPIJ
                SINIJ#SINIJ*EXPIJ

C            ACCUMULATE REQUIRED SUMS
  901        DADFI(I)#DADFI(I)+COSIJ
             DO 1101 K#1,3

 1101           DADX(K,I)#DADX(K,I)+HJ(K)*SINIJ

             IF(ITF-1)1501,1501,1301

 1301           DO 1401 K#1,6

 1401              DADB(K,I)#DADB(K,I)+HHJ(K)*COSIJ

C            BYPASS REMAINING SUMS IF CENTROSYMMETRIC
 1501        IF(ICENT-1)2201,2201,1601

 1601        DBDFI(I)#DBDFI(I)+SINIJ
             DO 1801 K#1,3

 1801           DBDX(K,I)#DBDX(K,I)+HJ(K)*COSIJ

             IF(ITF-1)2201,2201,2001

 2001           DO 2101 K#1,6

 2101              DBDB(K,I)#DBDB(K,I)+HHJ(K)*SINIJ

 2201        CONTINUE
C            END LOOP THROUGH THE NA ATOMS

 2301     CONTINUE
C         END LOOP THROUGH THE NS SYMMETRY TRANSFORMATIONS
```

```
C     COMPUTE A AND B AND THEIR DERIVATIVES                              FLS  775
      A#0.0                                                              FLS  776
      B#0.0                                                              FLS  777
      RHO#H(1)**2*PRCP(1)+H(2)**2*PRCP(2)+H(3)**2*PRCP(3)                FLS  778
     1   +2.0*H(1)*H(2)*PRCP(4)+2.0*H(1)*H(3)*PRCP(5)                   FLS  779
     2   +2.0*H(2)*H(3)*PRCP(6)                                         FLS  780
      IF(NF)2701,2801,2701                                               FLS  781
                                                                         FLS  782
 2701    SINTHL#SQRTF(RHO)                                               FLS  783
         PT#SINTHL/.05+1.0                                               FLS  784
         IPT#PT                                                          FLS  785
         FRACPT#PT-FLOATF(IPT)                                           FLS  786
                                                                         FLS  787
C     START LOOP THROUGH NA ATOMS                                        FLS  788
 2801 DO 5201 I#1,NA                                                     FLS  789
                                                                         FLS  790
C        OBTAIN SCATTERING FACTOR                                        FLS  791
         IF(NF)3101,3001,3101                                            FLS  792
                                                                         FLS  793
 3001       FI#SF(I)                                                     FLS  794
            GO TO 3201                                                   FLS  795
                                                                         FLS  796
 3101       L#SF(I)                                                      FLS  797
            FI#FX(IPT,L)+(FX(IPT+1,L)-FX(IPT,L))*FRACPT                  FLS  798
                                                                         FLS  799
C        COMPUTE ISOTROPIC TEMPERATURE FACTOR                            FLS  800
 3201    IF(ITF-1)3401,3401,3301                                         FLS  801
                                                                         FLS  802
 3301       TFI#1.0                                                      FLS  803
            GO TO 3501                                                   FLS  804
                                                                         FLS  805
 3401       TFI#EXPF(-BETA(I,I)*RHO)                                     FLS  806
                                                                         FLS  807
C        COMPUTE A AND ITS DERIVATIVES                                   FLS  808
 3501    FTA#FI*TFI*AI(I)                                                FLS  809
         FTACOS#FTA*DADFI(I)                                             FLS  810
         A#A+FTACOS                                                      FLS  811
         DADAI(I)#FI*TFI*DADFI(I)                                        FLS  812
         DADFI(I)#AI(I)*TFI*DADFI(I)                                     FLS  813
         PIFI#-6.28318531*FTA                                            FLS  814
         DO 3801 K#1,3                                                   FLS  815
                                                                         FLS  816
 3801       DADX(K,I)#PIFI*DADX(K,I)                                     FLS  817
                                                                         FLS  818
         IF(ITF-1)4201,4201,4001                                         FLS  819
                                                                         FLS  820
 4001       DO 4101 K#1,6                                                FLS  821
                                                                         FLS  822
 4101          DADB(K,I)#-FTA*DADB(K,I)                                  FLS  823
                                                                         FLS  824
            GO TO 4301                                                   FLS  825
                                                                         FLS  826
 4201       DADB(I,I)#-RHO*FTACOS                                        FLS  827
                                                                         FLS  828
C        COMPUTE B AND ITS DERIVATIVES UNLESS CENTROSYMMETRIC            FLS  829
 4301    IF(ICENT-1)5201,5201,4401                                       FLS  830
                                                                         FLS  831
 4401    FTASIN#FTA*DBDFI(I)                                             FLS  832
         B#B+FTASIN                                                      FLS  833
         DBDAI(I)#FI*TFI*DBDFI(I)                                        FLS  834
```

```
      DBDFI(I)#AI(I)*TFI*DBDFI(I)                                       FLS  835
      PIFI#-PIFI                                                        FLS  836
      DO 4701 K#1,3                                                     FLS  837
                                                                        FLS  838
 4701    DBDX(K,I)#PIFI*DBDX(K,I)                                       FLS  839
                                                                        FLS  840
      IF(ITF-1)5101,5101,4901                                           FLS  841
                                                                        FLS  842
 4901    DO 5001 K#1,6                                                  FLS  843
                                                                        FLS  844
 5001       DBDB(K,I)#-FTA*DBDB(K,I)                                    FLS  845
                                                                        FLS  846
         GO TO 5201                                                     FLS  847
                                                                        FLS  848
 5101    DBDB(1,I)#-RHO*FTASIN                                          FLS  849
                                                                        FLS  850
 5201 CONTINUE                                                          FLS  851
C     END LOOP THROUGH NA ATOMS                                         FLS  852
                                                                        FLS  853
C     CLEAR DERIVATIVES WITH RESPECT TO SCALE FACTORS                   FLS  854
 5301 DO 5302 I#1,NQ                                                    FLS  855
                                                                        FLS  856
 5302 DFDS(I)#0.0                                                       FLS  857
                                                                        FLS  858
C     COMPUTE SCALE FACTOR TIMES OVERALL TEMPERATURE FACTOR             FLS  859
      IQ#B(4)                                                           FLS  860
      SQTO#SC(IQ)*EXPF(-TO*RHO)                                         FLS  861
                                                                        FLS  862
C     CALCULATE F OR F**2 FOR CENTROSYMMETRIC OR NON-CENTROSYMMETRIC    FLS  863
C                                                                STRUCTURES FLS  864
      IF(IFSQ-1)5601,5601,6001                                          FLS  865
                                                                        FLS  866
 5601 IF(ICENT-1)5701,5701,5801                                         FLS  867
                                                                        FLS  868
 5701    CA#SIGNF(2.0*SQTO,A)                                           FLS  869
         CB#0.0                                                         FLS  870
         F#CA*A                                                         FLS  871
         GO TO 5901                                                     FLS  872
                                                                        FLS  873
 5801    SQRTAB#SQRTF(A**2+B**2)                                        FLS  874
         F#SQTO*SQRTAB                                                  FLS  875
         IF(SQRTAB)5807,5804,5807                                       FLS  876
                                                                        FLS  877
 5804       CA#0.0                                                      FLS  878
            CB#0.0                                                      FLS  879
            GO TO 5901                                                  FLS  880
                                                                        FLS  881
 5807    CA#SQTO*A/SQRTAB                                               FLS  882
         CB#SQTO*B/SQRTAB                                               FLS  883
                                                                        FLS  884
 5901 DFDS(IQ)#F/SC(IQ)                                                 FLS  885
 5902 DFDTO#-RHO*F                                                      FLS  886
      GO TO 6501                                                        FLS  887
                                                                        FLS  888
 6001 SQTO#SQTO**2                                                      FLS  889
      IF(ICENT-1)6201,6201,6301                                         FLS  890
                                                                        FLS  891
 6201    CA#8.0*SQTO*A                                                  FLS  892
         CB#0.0                                                         FLS  893
         F#CA*A/2.0                                                     FLS  894
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```
            GO TO 6401                                                  FLS  893
                                                                        FLS  894
 6301       F#SQTO*(A**2+B**2)                                          FLS  895
            CA#2.0*SQTO*A                                               FLS  896
            CB#2.0*SQTO*B                                               FLS  897
                                                                        FLS  898
 6401    DFDS(IQ)#2.0*F/SC(IQ)                                          FLS  899
         DFDTO#-2.0*RHO*F                                               FLS  900
                                                                        FLS  901
 6501 Y#F                                                               FLS  902
                                                                        FLS  903
C     COMPUTE DERIVATIVES OF F OR F**2                                  FLS  904
C     START LOOP THROUGH NA ATOMS                                       FLS  905
      DO 7501 I#1,NA                                                    FLS  906
                                                                        FLS  907
         DFDFI(I)#CA*DADFI(I)+CB*DBDFI(I)                               FLS  908
         DFDAI(I)#CA*DADAI(I)+CB*DBDAI(I)                               FLS  909
         DO 7001 K#1,3                                                  FLS  910
                                                                        FLS  911
 7001       DFDX(K,I)#CA*DADX(K,I)+CB*DBDX(K,I)                         FLS  912
                                                                        FLS  913
         IF(ITF-1)7201,7201,7301                                        FLS  914
                                                                        FLS  915
 7201       DFDB(1,I)#CA*DADB(1,I)+CB*DBDB(1,I)                         FLS  916
            GO TO 7501                                                  FLS  917
                                                                        FLS  918
 7301       DO 7401 K#1,6                                               FLS  919
                                                                        FLS  920
 7401          DFDB(K,I)#CA*DADB(K,I)+CB*DBDB(K,I)                      FLS  921
                                                                        FLS  922
 7501    CONTINUE                                                       FLS  923
C        END LOOP THROUGH NA ATOMS                                      FLS  924
                                                                        FLS  925
C     COPY DERIVATIVES INTO ARRAY DER WHICH IS THE SAME AS DC           FLS  926
      CALL SBTOP(DER,DFDS,DFDTO,DFDFI,DFDAI,DFDX,DFDB,ITF,NA,NG,NP)     FLS  927
      RETURN                                                            FLS  928
      END                                                               FLS  929


*TYPE(FORTRAN)                                                          FLS  930
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS  931
C     TEST FOR NON-POSITIVE-DEFINITE TEMPERATURE FACTORS                FLS  932
                                                                        FLS  933
      SUBROUTINE TEST                                                   FLS  934
                                                                        FLS  935
      COMMON NC,NV,NX,IW,IP,IT,NP,ISENT,NO,NM,NCY,IC,SIG,YC             FLS  936
      COMMON SQRTW,DY,WDY,JK,ISING,II,IID,PDI,IJ,IJD,PCLD               FLS  937
      COMMON SIGP,ISTOP,NT,NPCD,IXFE,HOLD,VARI                          FLS  938
      COMMON TITLE,P,X,YO,SIGYO,KI,SQSIG,AM,V,DC,DV,DIAC,PD,ROW         FLS 1938
      COMMON RNUM,RZNUM,RZDEN,WRNUM,WRZNUM,WRZDEN,R,RZ,WR,WRZ           FLS  939
      COMMON LABEL,ATOM,IHKL                                            FLS  940
      COMMON IFSQ,ITF,NF,NA,ICENT,NS,NC,TC,TJ,HX,HHB,EXPIJ,COSIJ,SINIJ  FLS  941
      COMMON FI,A,B,RHO,SINTHL,PT,IPT,FRACPT,FTA,FTACOS,FTASIN,TFI,PIFI FLS  942
      COMMON IQ,SQTO,SQRTAB,F,DFDTO                                     FLS  943
      COMMON SC,SF,AI,XYZ,BETA,DADFI,DBDFI,DADAI,DBDAI,DADX,DBDX,DADB   FLS  944
      COMMON DBDB,DFDS,DFDFI,DFDAI,DFDX,DFDB,IS,IS,HJ,HHJ,RCP,FX,PRCP   FLS  945
      COMMON CA,CB                                                      FLS  946
                                                                        FLS  947
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#230,NO(MAX)#2500,NX(MAX)#4,    FLS  948
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```
C        NF(MAX)#10,NA(MAX)#20,NS(MAX)#24,NQ(MAX)#9                      FLS  949
      DIMENSION TITLE(12),P(230),X(4,2500),YO(2500),SIGYO(2500),KI(230) FLS  950
      DIMENSION SQSIG(2),AM(5150),V(100),DC(230),DV(100)                FLS  951
      DIMENSION DIAG(100),PD(100),ROW(100),ATOM(20),LABEL(2,14),IHKL(4) FLS  952
      DIMENSION SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20),DADFI(20)     FLS  953
      DIMENSION DBDFI(20),DADAI(20),DBDAI(20),DADX(3,20),DBDX(3,20)     FLS  954
      DIMENSION DADB(6,20),DBDB(6,20),DFDS( 9),DFDFI(20),DFDAI(20)      FLS  955
      DIMENSION DFDX(3,20),DFDB(6,20),TS(3,24),IS(2,3,24),HJ(3),H(4)    FLS  956
      DIMENSION HHJ(6),RCP(6),FX(32,10),PRCP(6)                         FLS  957
                                                                        FLS  958
C     STORE ADJUSTED PARAMETERS IN VARIOUS ARRAYS                       FLS  959
      CALL PTOSB(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)                   FLS  960
                                                                        FLS  961
C     ENTER USERS SUBROUTINE TO RESET SYMMETRY-RELATED COORDINATES      FLS  962
      CALL RESETX(XYZ)                                                  FLS  963
                                                                        FLS  964
C     ENTER USERS SUBROUTINE TO RESET SYMMETRY-RELATED ANISOTROPIC      FLS  965
C                                   TEMPERATURE FACTOR COEFFICIENTS     FLS  966
      IF(ITF-1)60,60,50                                                 FLS  967
                                                                        FLS  968
   50    CALL RESETB(BETA)                                              FLS  969
                                                                        FLS  970
C     START LOOP THROUGH NA ATOMS                                       FLS  971
   60 DO 220 I#1,NA                                                     FLS  972
                                                                        FLS  973
   80    IF(ITF-1)100,90,100                                            FLS  974
                                                                        FLS  975
C           DISTRIBUTE OVERALL TEMPERATURE FACTOR AMONG ATOMS AND TEST  FLS  976
   90       BETA(1,I)#BETA(1,I)+TO                                      FLS  977
            IF(BETA(1,I))190,220,220                                    FLS  978
                                                                        FLS  979
  100       IF(TO)110,130,110                                           FLS  980
                                                                        FLS  981
C              DISTRIBUTE OVERALL TEMPERATURE FACTOR AMONG BETAS        FLS  982
  110          DO 120 K#1,6                                             FLS  983
                                                                        FLS  984
  120             BETA(K,I)#BETA(K,I)+TO*PRCP(K)                        FLS  985
                                                                        FLS  986
C           TEST ANISOTROPIC TEMPERATURE FACTOR COEFFICIENTS            FLS  987
  130       DO 145 K#1,3                                                FLS  988
                                                                        FLS  989
  140          IF(BETA(K,I))190,145,145                                 FLS  990
  145          CONTINUE                                                 FLS  991
                                                                        FLS  992
  150       IF(BETA(1,I)*BETA(2,I)-BETA(4,I)**2)190,160,160             FLS  993
                                                                        FLS  994
  160       IF(BETA(1,I)*BETA(3,I)-BETA(5,I)**2)190,170,170             FLS  995
                                                                        FLS  996
  170       IF(BETA(2,I)*BETA(3,I)-BETA(6,I)**2)190,180,180             FLS  997
                                                                        FLS  998
  180       IF(BETA(1,I)*BETA(2,I)*BETA(3,I)                            FLS  999
     1      +(BETA(4,I)*BETA(5,I)*BETA(6,I))*2.0                        FLS 1000
     2      -BETA(1,I)*BETA(6,I)**2-BETA(2,I)*BETA(5,I)**2              FLS 1001
     3      -BETA(3,I)*BETA(4,I)**2)190,220,220                         FLS 1002
                                                                        FLS 1003
C        PUT OUT ERROR STATEMENT                                        FLS 1004
  190    WRITE OUTPUT TAPE 9,200,I                                      FLS 1005
  200    FORMAT(28H0TEMPERATURE FACTOR OF ATOM I2,                      FLS 1006
     1      25H IS NOT POSITIVE-DEFINITE)                               FLS 1007
         ISTOP#1                                                        FLS 1008
```

```
  220     CONTINUE                                                      FLS 1009
C         END LOOP THROUGH NA ATOMS                                     FLS 1010
                                                                        FLS 1011
      TO#0.0                                                            FLS 1012
                                                                        FLS 1013
C     COPY PARAMETERS INTO THE ARRAY P                                  FLS 1014
      CALL SBTOP(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)                   FLS 1015
      RETURN                                                            FLS 1016
      END                                                               FLS 1017
                                                                        FLS 1018


*TYPE(FORTRAN)                                                          FLS 1019
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS 1020
C     COPY PARAMETERS FROM ARRAY P TO ARRAYS USED BY SUBROUTINES        FLS 1021
                                                                        FLS 1022
      SUBROUTINE PTOSB(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)             FLS 1023
      DIMENSION P(230),SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20)        FLS 1024
                                                                        FLS 1025
   10 I#1                                                               FLS 1026
   20 DO 40 J#1,NQ                                                      FLS 1027
                                                                        FLS 1028
   30    SC(J)#P(I)                                                     FLS 1029
   40    I#I+1                                                          FLS 1030
                                                                        FLS 1031
   50 TO#P(I)                                                           FLS 1032
   60 I#I+1                                                             FLS 1033
   70 DO 220 J#1,NA                                                     FLS 1034
                                                                        FLS 1035
   80    SF(J)#P(I)                                                     FLS 1036
   90    AI(J)#P(I+1)                                                   FLS 1037
  100    I#I+2                                                          FLS 1038
  110    DO 130 K#1,3                                                   FLS 1039
                                                                        FLS 1040
  120       XYZ(K,J)#P(I)                                               FLS 1041
  130       I#I+1                                                       FLS 1042
                                                                        FLS 1043
  140    IF(ITF-1)150,150,190                                           FLS 1044
                                                                        FLS 1045
  150       BETA(1,J)#P(I)                                              FLS 1046
  160       I#I+1                                                       FLS 1047
  170       GO TO 220                                                   FLS 1048
                                                                        FLS 1049
  190       DO 210 K#1,6                                                FLS 1050
                                                                        FLS 1051
  200          BETA(K,J)#P(I)                                           FLS 1052
  210          I#I+1                                                    FLS 1053
                                                                        FLS 1054
  220    CONTINUE                                                       FLS 1055
                                                                        FLS 1056
      RETURN                                                            FLS 1057
      END                                                               FLS 1058


*TYPE(FORTRAN)                                                          FLS 1059
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS 1060
C     COPY PARAMETERS FROM ARRAYS USED BY SUBROUTINES TO ARRAY P        FLS 1061
                                                                        FLS 1062
```

```
      SUBROUTINE SBTOP(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)
      DIMENSION P(230),SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20)

   10 I#1
   20 DO 40 J#1,NQ

   30    P(I)#SC(J)
   40    I#I+1

   50 P(I)#TO
   60 I#I+1
   70 DO 220 J#1,NA

   80    P(I)#SF(J)
   90    P(I+1)#AI(J)
  100    I#I+2
  110    DO 130 K#1,3

  120       P(I)#XYZ(K,J)
  130       I#I+1

  140    IF(ITF-1)150,150,190

  150       P(I)#BETA(1,J)
  160       I#I+1
  170       GO TO 220

  190       DO 210 K#1,6

  200          P(I)#BETA(K,J)
  210          I#I+1

  220    CONTINUE

      RETURN
      END


*TYPE(FAP)
       COUNT   230
       REM SYMMETRIC MATRIX INVERSE. SEE GLOSSARY FOR STORAGE SCHEME.
       REM FOR USE ON 704, 709, OR 7090.
       REM WRITTEN IN FAP FOR ASSEMBLY ON 709 OR 7090.
       ENTRY   SMI
 SMI   SXD T13,1
       SXD T14,2
       LFTM
       TNO *+1                        OVERFLOW TOGGLES
       CAL 1,4
       COM
       PAX 0,2
       TXI *+1,2,1
       CLA 2,4
       STA Y1
       CLA 3,4
       STA Y28
       STA SING1
 Y1    CLA 0                    ADD SET
       PDX 0,1
```

```
        STO Y27                                                 FLS 1120
        SXD T1,4                                                FLS 1121
Y2      SXD Y25,1          Y2                                   FLS 1122
        SXD T2,1                                                FLS 1123
        SXD T3,2                                                FLS 1124
        STZ T4             Y3                                   FLS 1125
        STZ T5,                                                 FLS 1126
        LXD T4,4                                                FLS 1127
Y4      SXD Y7,1           Y4                                   FLS 1128
        CLA 0,2            Y5                                   FLS 1129
        SSP                                                     FLS 1130
        FSB T4                                                  FLS 1131
        TMI Y7                                                  FLS 1132
        CLA 0,2            Y6                                   FLS 1133
        SSP                                                     FLS 1134
        STO T4                                                  FLS 1135
        SXD T5,4                                                FLS 1136
Y7      TIX Y8,2,0         Y7   DEC SET Y4,DELTA                FLS 1137
        HTR Y8                                                  FLS 1138
Y8      TNX Y10,1,1        Y8                                   FLS 1139
        TXI Y4,4,1         Y9                                   FLS 1140
Y10     CAL T3             Y10                                  FLS 1141
        ADD T2                                                  FLS 1142
        PDX 0,4                                                 FLS 1143
        CLA T5                                                  FLS 1144
        STO 0,4                                                 FLS 1145
        TSX X1,4           Y11                                  FLS 1146
        LXD T3,2           Y12                                  FLS 1147
        CLA 0,2                                                 FLS 1148
        TZE SING                                                FLS 1149
        TMI SING                                                FLS 1150
        CLA FLONE          Y13                                  FLS 1151
        FDP 0,2                                                 FLS 1152
        STQ 0,2                                                 FLS 1153
        CLS 0,2                                                 FLS 1154
        STO T6                                                  FLS 1155
        CLA PCN            Y14                                  FLS 1156
        SUB T3                                                  FLS 1157
        ARS 18                                                  FLS 1158
        STA Y16A                SETS ADDRESSES                  FLS 1159
        STA Y19                    AT M                         FLS 1160
        CLA PCN                                                 FLS 1161
        SUB T3                                                  FLS 1162
        ADD T2                                                  FLS 1163
        ARS 18                                                  FLS 1164
        STA Y16                 SETS ADDRESSES                  FLS 1165
        STA Y19A                   AT M+N                       FLS 1166
        LXD T2,1                                                FLS 1167
        LXD T2,2                                                FLS 1168
        CLA T3                                                  FLS 1169
        SUB T2                                                  FLS 1170
        PDX 0,4                                                 FLS 1171
Y15     TNX Y17,1,1        Y15                                  FLS 1172
Y16     LDQ 0,1            Y16  ADD SET Y14,M+N                 FLS 1173
        FMP T6                                                  FLS 1174
        TNO Y16A                                                FLS 1175
        SXD T12,4                                               FLS 1176
        TSX CFL,4                                               FLS 1177
        LXD T12,4                                               FLS 1178
Y16A    STO 0,1                 ADD SET Y14,M                   FLS 1179
```

```
DT1    TNX Y15,0,0                 DEC FOR T1,C(I4)                    FLS 1180
Y17    TNX Y24,2,1          Y17                                        FLS 1181
       PXD 0,2              Y18                                        FLS 1182
       PDX 0,1                                                         FLS 1183
Y19    LDQ 0,1              Y19  ADD SET Y14,M                         FLS 1184
Y19A   FMP 0,2                    ADD SET Y14,M+N                      FLS 1185
       TNO Y19B                                                        FLS 1186
       SXD T12,4                                                       FLS 1187
       TSX OFL,4                                                       FLS 1188
       LXD T12,4                                                       FLS 1189
Y19B   FAD 0,4                                                         FLS 1190
       TNO Y19C                                                        FLS 1191
       SXD T12,4                                                       FLS 1192
       TSX OFL,4                                                       FLS 1193
       LXD T12,4                                                       FLS 1194
Y19C   STO 0,4                                                         FLS 1195
       TXI Y20,4,-1                                                    FLS 1196
Y20    TNX Y17,1,1          Y20                                        FLS 1197
       TNX Y19,0,0                                                     FLS 1198
Y24    LXD T3,2             Y24                                        FLS 1199
       LXD T2,1                                                        FLS 1200
       TNX Y26,1,1                                                     FLS 1201
Y25    TIX Y2,2,0           Y25  DEC SET Y2                            FLS 1202
       HTR Y2                                                          FLS 1203
Y26    TXI Y26A,1,1         Y26                                        FLS 1204
Y26A   SXD Y29,1                                                       FLS 1205
Y27    TXL Y29,1,0          Y27  DEC SET Y1,0                          FLS 1206
       LXD T1,4             Y28                                        FLS 1207
       LXD T13,1                                                       FLS 1208
       LXD T14,2                                                       FLS 1209
Y28    STZ 0                ADD SET                                    FLS 1210
       EFTM                                                            FLS 1211
       TRA 4,4              NORMAL RETURN                              FLS 1212
Y29    TXI Y29A,2,0         Y29  DEC SET Y26                           FLS 1213
Y29A   SXD T3,2                                                        FLS 1214
       SXD T2,1                                                        FLS 1215
       CLA PON              Y30                                        FLS 1216
       SUB T3                                                          FLS 1217
       ARS 18                                                          FLS 1218
       STA Y35                     SETS ADDRESSES                      FLS 1219
       STA Y38                        AT M                             FLS 1220
       STA Y39                                                         FLS 1221
       STA Y39B                                                        FLS 1222
       STA Y39C                                                        FLS 1223
       CLA PON                                                         FLS 1224
       SUB T3                                                          FLS 1225
       ADD T2                                                          FLS 1226
       ARS 18                                                          FLS 1227
       STA Y31                     SETS ADDRESSES                      FLS 1228
       STA Y36                        AT M+N                           FLS 1229
       STA Y36A                                                        FLS 1230
       STA Y38B                                                        FLS 1231
       STA Y38C                                                        FLS 1232
       STA Y39A                                                        FLS 1233
       CLA T2                                                          FLS 1234
       SUB ONE                                                         FLS 1235
       PDX 0,1                     SETS INDEXES                        FLS 1236
       PDX 0,2                        AT M-N                           FLS 1237
Y31    STZ 0,1              Y31  ADD SET Y30,M+N                       FLS 1238
       TIX Y31,1,1          Y32                                        FLS 1239
```

```
        CLA T3                  Y33                                     FLS 1240
        SUB T2                                                          FLS 1241
        PDX 0,4                                                         FLS 1242
Y34     PXD 0,2                 Y34                                     FLS 1243
        PDX 0,1                                                         FLS 1244
Y35     LDQ 0,2                 Y35  ADD SET Y30,M                      FLS 1245
        FMP 0,4                                                         FLS 1246
        TNO Y36                                                         FLS 1247
        SXD T12,4                                                       FLS 1248
        TSX OFL,4                                                       FLS 1249
        LXD T12,4                                                       FLS 1250
Y36     FAD 0,1                 Y36  ADD SET Y30,M+N                    FLS 1251
        TNO Y36A                                                        FLS 1252
        SXD T12,4                                                       FLS 1253
        TSX OFL,4                                                       FLS 1254
        LXD T12,4                                                       FLS 1255
Y36A    STO 0,1                      ADD SET Y30,M+N                    FLS 1256
        TXI Y37,4,-1                                                    FLS 1257
Y37     TNX Y39,1,1             Y37                                     FLS 1258
Y38     LDQ 0,1                 Y38  ADD SET Y30,M                      FLS 1259
        FMP 0,4                                                         FLS 1260
        TNO Y38B                                                        FLS 1261
        SXD T12,4                                                       FLS 1262
        TSX OFL,4                                                       FLS 1263
        LXD T12,4                                                       FLS 1264
Y38B    FAD 0,2                      ADD SET Y30,M+N                    FLS 1265
        TNO Y38C                                                        FLS 1266
        SXD T12,4                                                       FLS 1267
        TSX OFL,4                                                       FLS 1268
        LXD T12,4                                                       FLS 1269
Y38C    STO 0,2                      ADD SET Y30,M+N                    FLS 1270
        TNX Y35,0,0                                                     FLS 1271
Y39     LDQ 0,2                 Y39  ADD SET Y30,M                      FLS 1272
Y39A    FMP 0,2                      ADD SET Y30,M+N                    FLS 1273
        TNO Y39B                                                        FLS 1274
        SXD T12,4                                                       FLS 1275
        TSX OFL,4                                                       FLS 1276
        LXD T12,4                                                       FLS 1277
Y39B    FAD 0                        ADD SET Y30,M                      FLS 1278
        TNO Y39C                                                        FLS 1279
        SXD T12,4                                                       FLS 1280
        TSX OFL,4                                                       FLS 1281
        LXD T12,4                                                       FLS 1282
Y39C    STO 0                        ADD SET Y30,M                      FLS 1283
        TIX Y34,2,1             Y40  GO TO Y50                          FLS 1284
        CAL T3                  Y50                                     FLS 1285
        ADD T2                                                          FLS 1286
        PDX 0,4                                                         FLS 1287
        CAL 0,4                                                         FLS 1288
        SLW T5                                                          FLS 1289
        TSX X1,4                Y51                                     FLS 1290
        LXD T3,2                Y52                                     FLS 1291
        LXD T2,1                                                        FLS 1292
DT12    TNX Y26,0,0                  DEC FOR T12                        FLS 1293
SING    PXD 0,2                 SINGULARITY RETURN                      FLS 1294
        LXD T13,1                                                       FLS 1295
        LXD T14,2                                                       FLS 1296
        LXD T1,4                                                        FLS 1297
        CLA ONE                                                         FLS 1298
SING1   STO 0                   ADD SET                                 FLS 1299
```

```
        EFTM                                                            FLS 1300
        TRA 4,4                 ERROR RETURN                            FLS 1301
OFL     ARS 1                   OVERFLOW-UNDERFLOW                      FLS 1302
        PBT                                                             FLS 1303
DT13    TNX OFL+5,0,0                 DEC FOR T13,C(I1)                 FLS 1304
        PXD 0,0,0                                                       FLS 1305
        TRA 1,4                                                         FLS 1306
        PXD 0,4                                                         FLS 1307
        SSM                                                             FLS 1308
DT14    TNX SING+1,0,0                DEC FOR T14,C(I2)                 FLS 1309
X1      CLA T5                  X1                                      FLS 1310
        TZE 1,4                                                         FLS 1311
        SXD T12,4               X2                                      FLS 1312
        LXD T2,1                                                        FLS 1313
        LXD T3,2                                                        FLS 1314
        CAL T3                                                          FLS 1315
        SUB T5                                                          FLS 1316
        PDX 0,4                                                         FLS 1317
        STD X6                                                          FLS 1318
X3      CAL 0,2                 X3                                      FLS 1319
        LDQ 0,4                                                         FLS 1320
        SLW 0,4                                                         FLS 1321
        STQ 0,2                                                         FLS 1322
        TNX X9,1,1              X4                                      FLS 1323
        SXD X8,1                X5                                      FLS 1324
X6      TXH X8,2,0              X6    DEC SET X2                        FLS 1325
        CAL ONE                 X7                                      FLS 1326
        STD X8                                                          FLS 1327
X8      TIX X8A,4,0             X8    DEC SET X5,X7                     FLS 1328
        HTR 0                                                           FLS 1329
X8A     TXI X3,2,-1                                                     FLS 1330
X9      LXD T3,2                X9                                      FLS 1331
        LXD X6,4                                                        FLS 1332
        CAL 0,2                                                         FLS 1333
        LDQ 0,4                                                         FLS 1334
        SLW 0,4                                                         FLS 1335
        STQ 0,2                                                         FLS 1336
        LXD T12,4               X10                                     FLS 1337
        TRA 1,4                                                         FLS 1338
ONE     PZE 0,0,1               ONE                                     FLS 1339
FLONE   DEC 1.0                 FLONE                                   FLS 1340
PON     PON 0,0,0               LGNO                                    FLS 1341
T2      PZE 0,0,0               T2, N                                   FLS 1342
T3      PZE 0,0,0               T3,-M                                   FLS 1343
T4      PZE 0,0,0               T4,X    T6,-B11                         FLS 1344
T5      PZE 0,0,0               T5,J                                    FLS 1345
T1      SYN DT1                 C(I4)                                   FLS 1346
T6      SYN T4                  -B11                                    FLS 1347
T12     SYN DT12                C(I4) FOR SR                            FLS 1348
T13     SYN DT13                C(I1)                                   FLS 1349
T14     SYN DT14                C(I2)                                   FLS 1350
        END 0                                                           FLS 1351


*TYPE(FORTRAN)                                                          FLS 1352
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                  FLS 1353
C       DUMMY SUBROUTINE TO BE REPLACED BY USER IF NECESSARY            FLS 1354
                                                                        FLS 1355
        SUBROUTINE PATCH(I,TJ,HJ,HNJ)                                   FLS 1356
```

```
      RETURN                                                            FLS 1357
      END                                                               FLS 1358


*TYPE(FORTRAN)                                                          FLS 1359
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS 1360
C     DUMMY SUBROUTINE TO BE REPLACED BY USER IF NECESSARY              FLS 1361
                                                                        FLS 1362
      SUBROUTINE RESETX(XYZ)                                            FLS 1363
      RETURN                                                            FLS 1364
      END                                                               FLS 1365


*TYPE(FORTRAN)                                                          FLS 1366
C     OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                    FLS 1367
C     DUMMY SUBROUTINE TO BE REPLACED BY USER IF NECESSARY              FLS 1368
                                                                        FLS 1369
      SUBROUTINE RESETB(BETA)                                           FLS 1370
      RETURN                                                            FLS 1371
      END                                                               FLS 1372
```

SUBROUTINES FOR EXAMPLE

```
*TYPE(FORTRAN)                                                          FLS 1373
C     EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.              FLS 1374
      SUBROUTINE PATCH(I,TJ,HJ,HHJ)                                     FLS 1375
      DIMENSION HJ(3),HHJ(6)                                            FLS 1376
                                                                        FLS 1377
C     BY-PASS MODIFICATION FOR FIRST ATOM                               FLS 1378
      IF(I-1)2,2,1                                                      FLS 1379
                                                                        FLS 1380
    1    HJ(1)#HJ(1)+HJ(2)                                              FLS 1381
         HJ(2)#0.0                                                      FLS 1382
         HHJ(1)#HHJ(1)+HHJ(2)                                           FLS 1383
         HHJ(2)#0.0                                                     FLS 1384
         HHJ(5)#HHJ(5)-HHJ(6)                                           FLS 1385
         HHJ(6)#0.0                                                     FLS 1386
                                                                        FLS 1387
    2 RETURN                                                            FLS 1388
      END                                                               FLS 1389


*TYPE(FORTRAN)                                                          FLS 1390
C     EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.              FLS 1391
      SUBROUTINE RESETX(XYZ)                                            FLS 1392
      DIMENSION XYZ(3,2)                                                FLS 1393
                                                                        FLS 1394
      XYZ(2,2)#XYZ(1,2)                                                 FLS 1395
                                                                        FLS 1396
      RETURN                                                            FLS 1397
      END                                                               FLS 1398


*TYPE(FORTRAN)                                                          FLS 1399
C     EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.              FLS 1400
      SUBROUTINE RESETB(BETA)                                           FLS 1401
```

```
      DIMENSION BETA(6,2)                                               FLS 1402
                                                                        FLS 1403
      BETA(2,2)#BETA(1,2)                                               FLS 1404
      BETA(6,2)#-BETA(5,2)                                              FLS 1405
                                                                        FLS 1406
      RETURN                                                            FLS 1407
      END                                                               FLS 1408
```

DATA FOR EXAMPLE

```
*DATA                                                                   FLS 1409
SCALE FACTOROVERALL B   FORM FACTOR MULTIPLIER  X            Y          FLS 1410
Z           BETA(1,1)   BETA(2,2)   BETA(3,3)   BETA(1,2)   BETA(1,3)   FLS 1411
BETA(2,3)   ATOMIC B                                                    FLS 1412
EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.                    FLS 1413
  2 15  1  0  0  0                                                      FLS 1414
  2  3  2  2  2  6  1                                                   FLS 1415
   10.000    9.551    8.475    7.159    5.908    4.857    4.028    3.394FLS 1416
    2.916    2.568    2.287    2.106    1.929    1.812    1.714    1.637FLS 1417
    1.574    1.515    1.469    1.425    1.381    1.339    1.299    1.259FLS 1418
    1.220    1.179    1.143    1.105    1.068    1.033    0.997    0.966FLS 1419
    10.00     9.95     9.79     9.54     9.20     8.79     8.33     7.83FLS 1420
     7.31     6.78     6.26     5.77     5.28     4.85     4.42     4.06FLS 1421
     3.71     3.42     3.13     2.90     2.68     2.50     2.33     2.19FLS 1422
     2.06     1.96     1.86        0        0        0        0        0FLS 1423
          1              2              3                                FLS 1424
         1-2            -2             -3                                FLS 1425
         2-1            -1   0.33333333+3                               FLS 1426
        -1               2-1 0.33333333-3                               FLS 1427
        -2               1-2 0.66666667+3                               FLS 1428
         2               1   0.66666667-3                               FLS 1429
 0.23504  0.23504  0.18504        0        0  0.50000                   FLS 1430
     1.0                                                                FLS 1431
       0                                                                FLS 1432
   0           1.       1.0   0.4100   0.2700   0.1200                  FLS 1433
    0.38                                                                FLS 1434
   SI          2.       0.5   0.5200   0.5200 .3333333                  FLS 1435
    0.43                                                                FLS 1436
       1        0        0    234.6                  1                  FLS 1437
       1        1        0    317.5                  1                  FLS 1438
       6        1        0     76.0                  1                  FLS 1439
       5        3        0     27.9                  1                  FLS 1440
       4        0        1    308.2                  1                  FLS 1441
       3        1        1     56.5                  1                  FLS 1442
       3        2        1      1.5                  1                  FLS 1443
       4        4        1      6.7                  1                  FLS 1444
       3        1       -1    199.8                  1                  FLS 1445
       5        2       -1    145.6                  1                  FLS 1446
       2        0        2     78.7                  1                  FLS 1447
       6        1        2     11.5                  1                  FLS 1448
       5        3        2     38.0                  1                  FLS 1449
       1        0       -2     80.1                  1                  FLS 1450
       5        1       -2     45.2                  1                  FLS 1451
       3        2       -2      9.0                  1                  FLS 1452
       3        0        3     74.1                  1                  FLS 1453
       2        2        3    212.0                  1                  FLS 1454
       3        0       -3     12.5                  1                  FLS 1455
       4        1       -3    231.3                  1                  FLS 1456
       6        0        4     44.4                  1                  FLS 1457
       6        2        4     32.0                  1                  FLS 1458
```

```
        5        0       -4    180.2                 1                FLS 1459
        4        2       -4     33.3                 1                FLS 1460
        1        1        5    162.5                 1                FLS 1461
        3        0       -5      8.2                 1                FLS 1462
        2        2        6     85.9                 1                FLS 1463
        4        0       -6    110.5                 1                FLS 1464
        4        1        7     10.6                 1                FLS 1465
        1        1       -7     78.0                 1                FLS 1466
        3        0        8    134.9                 1                FLS 1467
        2        1       -8     37.2                 1                FLS 1468
        2        0       -9     10.8                 1                FLS 1469
1                                                                    FLS 1470
1000111111111001001011 0                                             FLS 1471
```

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PROGRAM OUTPUT FOR EXAMPLE

```
EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

NUMBER OF CYCLES IN THIS JOB IS 2

NUMBER OF PARAMETERS TO BE VARIED IS  15

UNIT WEIGHTS TO BE SET BY PROGRAM

PARAMETERS TO BE READ AS INPUT DATA

CORRECTED PARAMETERS NOT TO BE SAVED FOR LATER USE

INPUT DATA FOR OR-FORTRAN FUNCTION AND ERROR PROGRAM NOT TO BE SAVED

BASED ON F SQUARED

ISOTROPIC TEMPERATURE FACTORS CONVERTED TO ANISOTROPIC BEFORE REFINING

NUMBER OF SCATTERING FACTOR TABLES IS  2

NUMBER OF ATOMS IN ASYMMETRIC UNIT IS  2

NON-CENTROSYMMETRIC

NUMBER OF SYMMETRY CARDS IS  6

NUMBER OF SCALE FACTORS IS  1

SCATTERING FACTOR TABLE  1

      10.000       9.551       8.475       7.159       5.908       4.857       4.028       3.394
       2.916       2.568       2.287       1.906       1.929       1.812       1.714       1.637
       1.574       1.515       1.469       1.425       1.381       1.339       1.299       1.259
       1.220       1.179       1.143       1.105       1.068       1.033       0.997       0.966

SCATTERING FACTOR TABLE  2

      10.000       9.950       9.790       9.540       9.200       8.790       8.330       7.830
       7.310       6.780       6.260       5.770       5.280       4.850       4.420       4.060
       3.710       3.420       3.130       2.900       2.680       2.500       2.330       2.190
       2.060       1.960       1.860       0.          0.          0.          0.          0.

SYMMETRY INFORMATION

     TRANSFORMED X            TRANSFORMED Y            TRANSFORMED Z

    -0.       1-0            -0.       2-0            -0.       3-0
    -0.       1-2            -0.      -2-0            -0.      -3-0
    -0.       2-1            -0.      -1-0             0.333333 3-0
    -0.      -1-0            -0.       2-1             0.333333-3-0
    -0.      -2-0            -0.       1-2             0.666667 3-0
    -0.       2-0            -0.       1-0             0.666667-3-0

RECIPROCAL CELL PARAMETERS     0.235040   0.235040   0.185040   0.         0.         0.500000

NUMBER OF PARAMETERS READ IS  24

NUMBER OF OBSERVATIONS READ IS   33

INPUT DATA
```

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I	P(I)	KI(I)
1	1.0000	1
2	0.	0
3	1.0000	0
4	1.0000	0
5	0.4100	1
6	0.2700	1
7	0.1200	1
8	0.0052	1
9	0.0052	1
10	0.0033	1
11	0.0026	1
12	0.	1
13	0.	1
14	2.0000	0
15	0.5000	0
16	0.5200	1
17	0.5200	0
18	0.3333	0
19	0.0059	1
20	0.0059	0
21	0.0037	1
22	0.0030	1
23	0.	1
24	0.	0

EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 1

H	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(O)	(O-C)/SIG(O)	IQ
1	0	0	234.6000	218.7436	-14.7900	-0.0000	15.8564	1.0000	15.8564	1
1	1	0	317.5000	407.2533	-17.1005	-10.7157	-89.7533	1.0000	-89.7533	1
6	1	0	76.0000	65.8654	-5.1086	-6.3062	10.1346	1.0000	10.1346	1
5	3	0	27.9000	13.7550	-1.5922	3.3496	14.1450	1.0000	14.1450	1
4	0	1	308.2000	201.8191	-7.1032	-12.3030	106.3809	1.0000	106.3809	1
3	1	1	56.5000	51.4033	-5.2238	4.9107	5.0967	1.0000	5.0967	1
3	2	1	1.5000	14.6171	-1.5141	-3.5106	-13.1171	1.0000	-13.1171	1
4	4	1	6.7000	4.4200	-1.8372	1.0220	2.2800	1.0000	2.2800	1
3	1	-1	199.8000	240.7640	-11.9863	-9.8536	-40.9640	1.0000	-40.9640	1
5	2	-1	145.6000	148.1294	-6.3258	10.3978	-2.5294	1.0000	-2.5294	1
2	0	2	78.7000	78.5276	4.4308	-7.6744	0.1724	1.0000	0.1724	1
6	1	2	11.5000	24.2969	4.6471	-1.6436	-12.7969	1.0000	-12.7969	1
5	3	2	38.0000	36.1203	0.7574	-5.9621	1.8797	1.0000	1.8797	1
1	0	-2	80.1000	69.5725	4.1705	7.2235	10.5275	1.0000	10.5275	1
5	1	-2	45.2000	59.9162	-3.8525	6.7137	-14.7162	1.0000	-14.7162	1
3	2	-2	9.0000	30.3347	-1.5878	-5.2739	-21.3347	1.0000	-21.3347	1
3	0	3	74.1000	90.0221	-9.4880	0.0000	-15.9221	1.0000	-15.9221	1
2	2	3	212.0000	252.9857	15.7640	2.1172	-40.9857	1.0000	-40.9857	1
3	0	-3	12.5000	1.2271	1.1077	-0.0000	11.2729	1.0000	11.2729	1
4	1	-3	231.3000	199.2133	-6.4939	-11.2739	32.0867	1.0000	32.0867	1
6	0	4	44.4000	20.2246	-2.2486	-3.8947	24.1754	1.0000	24.1754	1
6	2	4	32.0000	17.2503	-1.5961	-3.8344	14.7497	1.0000	14.7497	1
5	0	-4	180.2000	183.0317	-6.7645	11.7164	-2.8317	1.0000	-2.8317	1
4	2	-4	33.3000	21.6740	2.7004	-3.7924	11.6260	1.0000	11.6260	1
1	1	5	162.5000	160.0141	-9.0591	-8.8288	2.4859	1.0000	2.4859	1
3	0	-5	8.2000	19.6520	-2.2165	-3.8391	-11.4520	1.0000	-11.4520	1
2	2	6	85.9000	106.5043	10.3129	0.3856	-20.6043	1.0000	-20.6043	1
4	0	-6	110.5000	143.6837	11.9868	0.0000	-33.1837	1.0000	-33.1837	1
4	1	7	10.6000	12.7627	3.5417	-0.4681	-2.1627	1.0000	-2.1627	1
1	1	-7	78.0000	72.2755	-1.7725	-8.3147	5.7245	1.0000	5.7245	1
3	0	8	134.9000	132.1975	-5.7488	9.9573	2.7025	1.0000	2.7025	1
2	1	-8	37.2000	37.1470	6.0147	0.9850	0.0530	1.0000	0.0530	1
2	0	-9	10.8000	14.9334	3.8644	0.0000	-4.1334	1.0000	-4.1334	1

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 0.2852E 05

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 39.8081

	NUMERATOR	DENOMINATOR	R
R FACTOR INCLUDING ZEROS	597.837	3095.200	0.193
R FACTOR OMITTING ZEROS	597.837	3095.200	0.193
WEIGHTED R FACTOR INCLUDING ZEROS	168.892	742.077	0.228
WEIGHTED R FACTOR OMITTING ZEROS	168.892	742.077	0.228

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EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

PARAMETER	OLD	CHANGE	NEW	ERROR
SCALE FACTOR	1.0000000	0.0005857	1.0005857	0.0064983
OVERALL B	0.		0.	
O				
FORM FACTOR	1.0000000		1.0000000	
MULTIPLIER	1.0000000		1.0000000	
X	0.4100000	0.0053155	0.4153155	0.0006499
Y	0.2700000	-0.0023085	0.2676915	0.0008087
Z	0.1200000	-0.0025466	0.1174534	0.0006581
BETA(1,1)	0.0052482	-0.0026719	0.0025762	0.0023483
BETA(2,2)	0.0052482	-0.0019391	0.0033091	0.0022263
BETA(3,3)	0.0032528	-0.0005468	0.0027060	0.0007256
BETA(1,2)	0.0026241	-0.0028966	-0.0002725	0.0016950
BETA(1,3)	0.	-0.0009170	-0.0009170	0.0010200
BETA(2,3)	0.	0.0003482	0.0003482	0.0008362
SI				
FORM FACTOR	2.0000000		2.0000000	
MULTIPLIER	0.5000000		0.5000000	
X	0.5200000	0.0088597	0.5288597	0.0003916
Y	0.5200000		0.5200000	
Z	0.3333333		0.3333333	
BETA(1,1)	0.0059387	0.0033190	0.0092577	0.0006799
BETA(2,2)	0.0059387		0.0059387	
BETA(3,3)	0.0036808	0.0004300	0.0041108	0.0003421
BETA(1,2)	0.0029693	0.0041426	0.0071120	0.0011583
BETA(1,3)	0.	0.0004649	0.0004649	0.0004607
BETA(2,3)	0.		0.	

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

SUM(W*(O-C)**2) IS 0.3070E 03

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 4.1300

EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 2

H	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(O)	(O-C)/SIG(O)	IQ
1	0	0	234.6000	232.7308	-15.2466	-0.0000	1.8692	1.0000	1.8692	1
1	1	0	317.5000	327.9457	-16.4159	-7.6210	-10.4457	1.0000	-10.4457	1
6	1	0	76.0000	68.1950	-4.6793	-6.7985	7.8050	1.0000	7.8050	1
5	3	0	27.9000	23.2770	-1.9372	4.4155	4.6230	1.0000	4.6230	1
4	0	1	308.2000	312.7573	-8.8373	-15.3066	-4.5573	1.0000	-4.5573	1
3	1	1	56.5000	48.8201	-5.1902	4.6717	7.6799	1.0000	7.6799	1
3	2	1	1.5000	2.0536	-1.2360	-0.7236	-0.5536	1.0000	-0.5536	1
4	4	1	6.7000	3.3605	-1.7412	-0.5698	3.3395	1.0000	3.3395	1
3	1	-1	199.8000	201.2066	-11.1717	-8.7272	-1.4066	1.0000	-1.4066	1
5	2	-1	145.6000	140.7784	-6.7253	9.7665	4.8216	1.0000	4.8216	1
2	0	2	78.7000	73.1369	4.2735	-7.4019	5.5631	1.0000	5.5631	1
6	1	2	11.5000	16.0669	2.7012	-2.9583	-4.5669	1.0000	-4.5669	1
5	3	2	38.0000	34.8800	1.7165	-5.6474	3.1200	1.0000	3.1200	1
1	0	-2	80.1000	84.4342	4.5917	7.9531	-4.3342	1.0000	-4.3342	1
5	1	-2	45.2000	44.0862	-2.4543	6.1653	1.1138	1.0000	1.1138	1
3	2	-2	9.0000	13.2939	-2.0058	-3.0422	-4.2939	1.0000	-4.2939	1
3	0	3	74.1000	75.0796	-8.6598	0.0000	-0.9796	1.0000	-0.9796	1
2	2	3	212.0000	211.9543	14.4354	1.8239	0.0457	1.0000	0.0457	1
3	0	-3	12.5000	13.4910	3.6709	-0.0000	-0.9910	1.0000	-0.9910	1
4	1	-3	231.3000	222.6483	-8.0450	-12.5565	8.6517	1.0000	8.6517	1
6	0	4	44.4000	45.3348	-3.3646	-5.8276	-0.9348	1.0000	-0.9348	1
6	2	4	32.0000	29.3684	-1.4792	-5.2102	2.6316	1.0000	2.6316	1
5	0	-4	180.2000	170.2345	-6.5199	11.2928	9.9655	1.0000	9.9655	1
4	2	-4	33.3000	28.9555	3.4983	-4.0846	4.3445	1.0000	4.3445	1
1	1	5	162.5000	162.6359	-9.2383	-8.7806	-0.1359	1.0000	-0.1359	1
3	0	-5	8.2000	7.8908	-1.4037	-2.4313	0.3092	1.0000	0.3092	1
2	2	6	85.9000	87.2194	9.3150	0.5905	-1.3194	1.0000	-1.3194	1
4	0	-6	110.5000	107.7816	10.3757	0.0000	2.7184	1.0000	2.7184	1
4	1	7	10.6000	10.4373	3.1009	-0.8997	0.1627	1.0000	0.1627	1
1	1	-7	78.0000	75.4176	-1.8850	-8.4721	2.5824	1.0000	2.5824	1
3	0	8	134.9000	133.1443	-5.7660	9.9871	1.7557	1.0000	1.7557	1
2	1	-8	37.2000	35.5399	5.8589	1.0826	1.6601	1.0000	1.6601	1
2	0	-9	10.8000	12.6012	3.5477	0.0000	-1.8012	1.0000	-1.8012	1

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 2

SUM(W*(O-C)**2) IS 0.6391E 03

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 5.9588

	NUMERATOR	DENOMINATOR	R
R FACTOR INCLUDING ZEROS	111.083	3095.200	0.036
R FACTOR OMITTING ZEROS	111.083	3095.200	0.036
WEIGHTED R FACTOR INCLUDING ZEROS	25.281	742.077	0.034
WEIGHTED R FACTOR OMITTING ZEROS	25.281	742.077	0.034

EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

PARAMETERS AFTER LEAST SQUARES CYCLE 2

PARAMETER	OLD	CHANGE	NEW	ERROR
SCALE FACTOR	1.0005857	-0.0002306	1.0003550	0.0030914
OVERALL B	0.		0.	
O				
FORM FACTOR	1.0000000		1.0000000	
MULTIPLIER	1.0000000		1.0000000	
X	0.4153155	0.0002572	0.4155727	0.0002937
Y	0.2676915	-0.0000361	0.2676554	0.0003717
Z	0.1174534	0.0005464	0.1179998	0.0003146
BETA(1,1)	0.0025762	0.0013604	0.0039366	0.0009567
BETA(2,2)	0.0033091	0.0012008	0.0045099	0.0009366
BETA(3,3)	0.0027060	0.0000222	0.0027282	0.0003574
BETA(1,2)	-0.0002725	0.0022977	0.0020252	0.0007473
BETA(1,3)	-0.0009170	0.0009445	0.0000276	0.0004045
BETA(2,3)	0.0003482	-0.0001149	0.0002333	0.0003995
SI				
FORM FACTOR	2.0000000		2.0000000	
MULTIPLIER	0.5000000		0.5000000	
X	0.5288597	0.0006168	0.5294765	0.0001849
Y	0.5288597		0.5288597	
Z	0.3333333		0.3333333	
BETA(1,1)	0.0092577	-0.0025950	0.0066626	0.0003353
BETA(2,2)	0.0092577		0.0092577	
BETA(3,3)	0.0041108	-0.0000992	0.0040116	0.0001728
BETA(1,2)	0.0071120	-0.0036885	0.0034235	0.0005486
BETA(1,3)	0.0004649	-0.0002781	0.0001868	0.0001929
BETA(2,3)	-0.0004649		-0.0004649	

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 2

SUM(W*(O-C)**2) IS 0.6423E 02

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 1.8890

EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 3

H	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(O)	(O-C)/SIG(O)	IQ
1	0	0	234.6000	234.1317	-15.2959	0.	0.4683	1.0000	0.4683	1
1	1	0	317.5000	317.0131	-16.2133	-7.3428	0.4869	1.0000	0.4869	1
6	1	0	76.0000	77.7327	-4.5320	-7.5590	-1.7327	1.0000	-1.7327	1
5	3	0	27.9000	28.2317	-1.5830	5.0681	-0.3317	1.0000	-0.3317	1
4	0	1	308.2000	308.9362	-8.7852	-15.2164	-0.7362	1.0000	-0.7362	1
3	1	1	56.5000	54.8334	-5.6606	4.7699	1.6666	1.0000	1.6666	1
3	2	1	1.5000	0.8846	-0.8137	-0.4710	0.6154	1.0000	0.6154	1
4	4	1	6.7000	5.3824	-2.2270	-0.6472	1.3176	1.0000	1.3176	1
3	1	-1	199.8000	199.6167	-11.0970	-8.7368	0.1833	1.0000	0.1833	1
5	2	-1	145.6000	147.9503	-8.8145	10.0702	-2.3503	1.0000	-2.3503	1
2	0	2	76.7000	76.9905	4.3857	-7.5962	1.7095	1.0000	1.7095	1
6	1	2	11.5000	10.3763	1.8161	-2.6591	1.1237	1.0000	1.1237	1
5	3	2	38.0000	37.2095	2.0457	-5.7444	0.7905	1.0000	0.7905	1
1	0	-2	80.1000	83.8707	4.5774	7.9283	-3.7707	1.0000	-3.7707	1
5	1	-2	45.2000	44.2917	-2.8921	5.9915	0.9083	1.0000	0.9083	1
3	2	-2	9.0000	9.9462	-1.3176	-2.8641	-0.9462	1.0000	-0.9462	1
3	0	3	74.1000	75.2471	-8.6714	0.0000	-1.1471	1.0000	-1.1471	1
2	2	3	212.0000	214.3139	14.4598	2.2528	-2.3139	1.0000	-2.3139	1
3	0	-3	12.5000	12.2621	3.5005	-0.0000	0.2379	1.0000	0.2379	1
4	1	-3	233.3000	231.6780	-8.0738	-12.8966	-0.3780	1.0000	-0.3780	1
6	0	4	44.4000	45.9496	-3.3861	-5.8684	-1.5496	1.0000	-1.5496	1
6	2	4	32.0000	30.1678	-1.1340	-5.3722	1.8322	1.0000	1.8322	1
5	0	-4	180.2000	180.1200	-6.7081	11.6187	0.0800	1.0000	0.0800	1
4	2	-4	33.3000	32.3981	3.8084	-4.2274	0.9019	1.0000	0.9019	1
1	1	5	162.5000	161.5392	-9.2103	-8.7519	0.9608	1.0000	0.9608	1
3	0	-5	8.2000	7.3109	-1.3515	-2.3408	0.8891	1.0000	0.8891	1
2	2	5	85.9000	86.7965	9.2960	0.5654	-0.8965	1.0000	-0.8965	1
4	0	-6	110.5000	109.9934	10.4841	0.0000	0.5066	1.0000	0.5066	1
4	1	7	10.6000	11.9148	3.3502	-0.8260	-1.3148	1.0000	-1.3148	1
1	1	-7	78.0000	75.7974	-1.6880	-8.5378	2.2026	1.0000	2.2026	1
3	0	8	134.9000	135.9982	-5.8288	10.0959	-1.0982	1.0000	-1.0982	1
2	1	-8	37.2000	37.1921	5.9645	1.2612	0.0079	1.0000	0.0079	1
2	0	-9	10.8000	12.8688	3.5860	0.0000	-2.0688	1.0000	-2.0688	1

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 3

SUM(W*(O-C)**2) IS 0.63588 D2

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 1.8795

	NUMERATOR	DENOMINATOR	R
R FACTOR INCLUDING ZEROS	37.504	3095.200	0.012
R FACTOR OMITTING ZEROS	37.504	3095.200	0.012
WEIGHTED R FACTOR INCLUDING ZEROS	7.974	742.077	0.011
WEIGHTED R FACTOR OMITTING ZEROS	7.974	742.077	0.011

EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.

CORRELATION MATRIX

1	1.0000	-0.2333	-0.4564	0.3507	0.3961	0.1185	0.1093	0.2206	0.3141	-0.0880
	0.3056	0.1460	0.0384	-0.1757	-0.0327					
2	0.	1.0000	0.6823	-0.3275	-0.1397	0.2778	-0.0905	0.3230	-0.2742	-0.0365
	-0.1273	0.0795	0.3163	0.3530	-0.1876					
3	0.	0.	1.0000	-0.4928	0.0294	0.0029	-0.0474	0.2678	-0.3861	-0.1187
	-0.1731	-0.0925	0.3310	0.2453	-0.0533					
4	0.	0.	0.	1.0000	-0.2308	-0.0646	0.2524	-0.3875	0.5313	0.1682
	0.3611	0.0214	-0.2946	-0.3009	-0.1763					
5	0.	0.	0.	0.	1.0000	-0.3491	-0.1624	0.4986	0.0317	-0.3117
	-0.0437	0.1582	0.2053	0.1425	-0.0606					
6	0.	0.	0.	0.	0.	1.0000	-0.1114	0.4683	-0.1232	0.2852
	0.1512	-0.1383	0.1851	0.0651	0.0631					
7	0.	0.	0.	0.	0.	0.	1.0000	-0.1634	0.1426	0.0746
	0.2481	-0.0295	-0.6210	-0.2146	-0.0209					
8	0.	0.	0.	0.	0.	0.	0.	1.0000	-0.1179	-0.0091
	-0.1230	0.2205	0.3056	0.3943	-0.0921					
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.1294
	0.3157	0.0340	-0.1717	-0.2362	-0.1875					
10	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000
	-0.0816	0.0905	-0.0478	0.0514	0.1900					
11	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
	1.0000	-0.3190	-0.1875	-0.4356	-0.1780					
12	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
	0.	1.0000	-0.1099	0.8212	-0.2014					
13	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
	0.	0.	1.0000	0.1563	-0.0327					
14	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	1.0000	-0.2221					
15	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	1.0000					

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OR FFE,

A FORTRAN CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM

W. R. Busing
K. O. Martin
H. A. Levy

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OR FFE,

A FORTRAN CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM

by

W. R. Busing, K. O. Martin, and H. A. Levy
Chemistry Division and Mathematics Division

MARCH 1964

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ABSTRACT

This report describes a computer program which calculates interatomic distances, bond angles, principal axes of thermal motion, and other functions of the unit cell parameters, the atomic coordinates, and the temperature factor coefficients of a crystal structure. The standard errors of these functions are computed from the variance-covariance matrix of the parameters if this is known. The program may be used independently, or the input may be taken from a magnetic tape prepared by the crystallographic least-squares program OR FLS.

The program is written entirely in Fortran, and detailed instructions for its use are included. The necessary card decks may be obtained from the authors.

INTRODUCTION

Given the unit cell parameters of a crystal together with the atomic coordinates and/or the anisotropic temperature factor coefficients, this program computes various functions of these parameters, such as the distance between two atoms, an angle defined by three atoms, the principal axes of the anisotropic temperature factor, etc. If the errors of the input parameters are available to the program in the form of a variance-covariance matrix obtained, for example, from the inverse matrix of a least squares refinement, the program will also compute the standard errors of the functions with and without the contribution of the cell parameter errors. This program may be used independently, with all input data read from cards, or it may be used in conjunction with the least squares refinement program OR FLS, in which case much of the input is taken from a magnetic tape produced by that program.

The types of functions which can be evaluated are defined by subroutines, of which fifteen are included in the present program. The detailed specification of each function or group of functions to be computed is made by means of an instruction card which will be described below. If functions are desired other than those already included, the user need only write a Fortran II subroutine for the function, compile it, and add it to the deck. To facilitate such programming, several subroutines for the manipulation of matrices and vectors are included in the program, and descriptions of these

will be given below together with detailed specifications for writing subroutines for new functions.

This program is a revision of the earlier OR XFE (W. R. Busing and H. A. Levy, "A Crystallographic Function and Error Program for the IBM 704," ORNL-CF 59-12-3 (1959)). It is now written entirely in Fortran II and comments have been added to facilitate any modification which may be desired. Card decks are available from the authors on request.

MATHEMATICAL METHOD

The functions which the program computes are of the form

$$f = f(p_1, p_2, p_3 \ldots\ldots a_1, a_2 \ldots\ldots a_6)$$

where the p's are the atomic parameters and the a's are the unit cell parameters. Each kind of function is computed by a special subroutine for this purpose, and the mathematical expressions used are best obtained from the Fortran language listings of these subroutines designated FUN1, FUN2, etc.

The standard error of f is given by

$$e = (e'^2 + e''^2)^{1/2}$$

where

$$e'^2 = \sum_{j=i}^{n} \sum_{i=1}^{n} C_{ij} \left(\frac{\partial f}{\partial p_i}\right) \left(\frac{\partial f}{\partial p_j}\right) V_{ij}$$

and

$$e''^2 = \sum_{j=i}^{6} \sum_{i=1}^{6} C_{ij} \left(\frac{\partial f}{\partial a_i}\right) \left(\frac{\partial f}{\partial a_j}\right) U_{ij}.$$

Here V_{ij} is an element of the variance-covariance matrix which describes the errors of the atomic parameters, and U_{ij} is an element of a similar matrix for the unit cell parameters. $C_{ij} = 1$ if $i = j$; otherwise $C_{ij} = 2$.

When errors are to be computed the user has the option of obtaining $\underset{\sim}{V}$ from a tape produced by OR FLS. In this case the program stores

$$V_{ij} = [\Sigma w(\text{OBS} - \text{CALC})^2/(m-n)]\ b_{ij}$$

where b_{ij} is an element of the inverse matrix of the normal equations, and the constant in brackets is the weighted sum of the squares of the residuals divided by the number of degrees of freedom. The other option available to the user is to read V_{ij} directly from cards.

The unit cell errors may be put in in two ways. If no covariances are known then the user may supply the six standard errors $\sigma(a_i)$. The program then sets

$$U_{ii} = \sigma^2(a_i)$$

$$U_{ij} = 0,\ i \neq j.$$

Alternatively the 21 independent values of U_{ij} $(i \leq j)$ can be read from cards.

The necessary derivatives are computed numerically by adding an increment Δp_i to p_i and re-entering the subroutine for f. The derivative is then

$$\frac{\partial f}{\partial p_i} \approx \frac{f(p_1, p_2, .., p_i + \Delta p_i, .., a_1, ...) - f(p_1, p_2, .., p_i, .., a_1, ...)}{\Delta p_i}.$$

The increment used is $\Delta p_i = (0.01)V_{ii}^{1/2}$. The derivatives

with respect to the cell parameters are obtained similarly.

The program is arranged so that it computes derivatives only with respect to the parameters actually involved in f. The information as to which these are is provided by the subroutines PRE1, PRE2, etc., which are supplied for each type of function. Derivative computations are also omitted with respect to fixed parameters which are not represented in the variance-covariance matrix. If this situation arises because certain atoms are in special positions, then the errors are computed correctly. However, if parameters have been fixed for other reasons, it is possible that important terms are omitted from the calculated errors.

Note that for the derivative computation to be correct all symmetry transformations must be made after Δp_i has been added to p_i. Similarly all constraints on the parameters must be set after incrementing. (See the section entitled "Constraints on the Parameters".) In other words, the function f is always computed directly from the fundamental parameters, the errors of which are described by the matrices $\underset{\sim}{V}$ and $\underset{\sim}{U}$.

The output of the program includes a description of the function, the value f of the function, the standard error e of the function, and the standard error e' not including the effect of unit cell errors.

CONSTRAINTS ON THE PARAMETERS

In order to insure that this program correctly computes the errors of various functions, it is necessary for the user to consider whether the symmetry of the crystal introduces constraints either on the cell parameters, a_i, or on the atomic parameters, p_i. A simple case occurs when the symmetry forces a parameter to have a fixed value, and this situation is correctly treated by specifying that the error of this parameter is zero. A more complicated procedure is required when the symmetry imposes a relationship between two or more parameters. In this case one of the interrelated parameters is chosen as independent and a Fortran II subroutine is written to set the values of the dependent parameters in terms of it. The main program will enter this subroutine immediately before each entry to the function-computing subroutine so that the derivatives needed for the error calculation are correctly computed. In the input data the errors associated with the dependent parameters should be set to zero. (When the atomic parameters are taken from a least-squares refinement these errors are automatically zero, since the dependent parameters would not have been varied.)

Specifications are given here for subroutines SETA and SETP which establish these constraints, and examples are included in the sample calculations. The statements required are summarized as follows:

```
SUBROUTINE SETA(A)
DIMENSION A(6)
Include statements to set the values of the A(I)'s
which are taken as dependent in terms of those chosen
as independent.
RETURN
END
SUBROUTINE SETP(P)
DIMENSION P(300)
Include statements to set the values of the P(I)'s
which are taken as dependent in terms of those chosen
as independent.
RETURN
END
```

These routines should be compiled and substituted in the binary deck for the dummy routines with the same names.

ATOM DESIGNATION AND SYMMETRY TRANSFORMATIONS

In the course of preparing an instruction card to specify a function to be computed, it will be necessary to define the one or more atoms involved in this function. This is done by means of an atom designation consisting of the two integers a and 100c + s. Here a = 1, 2, 3, ... is the number of the atom in the parameter list, s = 0, 1, 2, ... is the number of the symmetry transformation to be applied, and c = 0, 1, ... 7 defines the unit cell translations as described below.

The program obtains the coordinates of an atom in the following way:

1. The integer a is used to compute the location of the coordinates in the parameter list and x, y, z are picked up. If a = 0 the program sets x = y = z = 0.

2. These coordinates are then transformed to x', y', z' according to the symmetry information punched on symmetry card s. If s = 0 no transformation is made.

3. The cell translations are then made according to the following table:

c	z''	y''	x''
0	z'	y'	x'
1	z'	y'	$x' - 1$
2	z'	$y' - 1$	x'
3	z'	$y' - 1$	$x' - 1$
4	$z' - 1$	y'	x'
5	$z' - 1$	y'	$x' - 1$
6	$z' - 1$	$y' - 1$	x'
7	$z' - 1$	$y' - 1$	$x' - 1$

(As a memory aid, note that the 1's in this table correspond to the binary representation of c.)

For example, atom (3,208) is atom 3 in the parameter list transformed to symmetry position 8 of cell 2, while atom (5,0) is atom 5 just as it appears in the list of parameters. In a subsequent section we will refer to atom 3 in asymmetric unit 208 or atom 5 in the basic asymmetric unit (unit 0).

Note that transformations such as $x' = -x$ and $x' = 1-x$ are not in general equivalent for purposes of this program.

The program obtains the matrix of the anisotropic temperature factor coefficients of an atom in a similar way except that the elements of this matrix are transformed as the corresponding products of the coordinates. This procedure is valid for an atom in either a special or general position provided that the symmetry cards are written for general positions. (See H. A. Levy, Acta Cryst. (1956). 9, 679). The translational part of the symmetry transformation is irrelevant in this case as is the cell translation c. If a = 0, a null matrix will be generated.

DATA INPUT

1. Title card. FORMAT(12A6)

Columns	
1-72	Title consisting of any desired Hollerith information. This will be printed unchanged on the output.

2. Control card. FORMAT(9I3)

Columns	
1-3	IPM, the atomic parameter error indicator. The variance-covariance matrix and parameter selection information will (IPM = 0) not be used. (IPM = 1) be used to compute errors.
4-6	NP, the input indicator. If NP = 0, the structure parameters will be read from the private tape written by OR FLS. (If the variance-covariance matrix and parameter selection information are to be used, they will also be read from this tape when NP = 0). If NP > 0, data will be taken entirely from cards, and NP is equal to the number of structure parameters to be read from the cards. $0 \leqslant NP \leqslant 300.$

Columns

7-9 IAM, the cell parameter error indicator. The cell parameter errors are
(IAM = 0) not to be used.
(IAM = 1) to be read in the form of standard errors.
(IAM = 2) to be read in the form of a variance-covariance matrix.

10-12 NS, the number of symmetry cards to be read.

$0 \leqslant NS \leqslant 48.$

13-15 NV, the order of the variance-covariance matrix, PM, if it is to be read from cards. If the matrix is to be read from the OR FLS tape, NV will also be read from this tape and this field is irrelevant. If the variance-covariance matrix is not to be used, set NV = 0.

$0 \leqslant NV \leqslant 200.$

The following parameter arrangement integers must be supplied if the structure parameters are read from cards. They are supplied automatically by the program if the parameters are read from the private output tape of OR FLS. For more details see 3 below.

Columns

16-18 JXP, the period of the position parameters in the parameter list. If no position parameters are included in the list, set JXP and JX = 0.

19-21 JX, the position of the first x coordinate in the parameter list.

22-24 JBP, the period of the temperature factor coefficients in the parameter list. If no temperature factor coefficients are included in the list, set JBP and JB = 0.

25-27 JB, the position of the first temperature factor coefficient in the parameter list.

3. Atomic parameter cards. FORMAT(8F9.4)
If NP = 0, the atomic parameters will be read from the private output tape of OR FLS, and the atomic parameter cards are omitted from the card input. Otherwise NP parameters must be punched eight per card. The arrangement of these parameters is subject to the following restrictions:

a) For each atom the position parameters x, y, z must be in sequence.

b) Position parameters for successive atoms must appear periodically in the order of the atom designation.

c) If anisotropic temperature factor coefficients are included, they must be in the sequence β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}, for each atom. These β's are defined by the following expression for the temperature factor:

$$\exp[-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})].$$

d) Temperature factor coefficients of successive atoms must appear periodically in the order of the atom designation.

Thus the position parameters of atom I start with P(J) where J = JXP*(I-1) + JX, and the temperature factor coefficients of atom I start with P(K) where K = JBP*(I-1) + JB.

4. Parameter selection cards. FORMAT(72I1)
The purpose of these cards is to identify those parameters which are associated with the elements of the variance-covariance matrix PM. They are exactly the same as the parameter selection cards used with OR FLS.

These cards are not to be supplied unless the control card integers IPM and NP specify that the variance-covariance matrix and parameter selection information will be used and will be read from cards (IPM = 1 and NP > 0).

Each column of a parameter selection card corresponds to one parameter. The first card is associated with parameters 1 to 72, the second with parameters 73 to 144, etc. If a parameter is represented in the matrix a one is punched in the corresponding column; otherwise a zero or blank is punched. The total number of one punches must be equal to NV, the order of the matrix. The first parameter in the list for which a one punch is found is assumed to correspond to the first row and column of the matrix, the second with the second, etc.

5. Variance-covariance matrix, PM, for structure parameters. FORMAT(6E12.6)
These cards are to be supplied only if the variance-covariance matrix is to be used and is to be read from cards (IPM = 1 and NP > 0).

First card
Columns
1-12 A scale factor by which the matrix will be multiplied. This could be unity or $\Sigma w(F_o - F_c)^2/(m - n)$, for example.

Subsequent cards
The NV(NV + 1)/2 unique elements of the matrix PM punched six per card in the order PM(1,1), PM(1,2),....., PM(1,NV), PM(2,2), PM(2,3),...., PM(2,NV), PM(3,3),...., PM(NV,NV), where NV is the order of the matrix. The parameters with which this matrix is associated are defined by the parameter selection cards.

6. Cell parameter card. FORMAT(6F9.4)
These six direct unit cell parameters must always be supplied.

Columns	
1-9	A(1) = a
10-18	A(2) = b
19-27	A(3) = c
28-36	A(4) = cos α
37-45	A(5) = cos β
46-54	A(6) = cos γ

7. Cell parameter error cards.
If the effect of the cell parameter errors is not to be considered (IAM = 0), these cards are omitted. If it is to be included, the cell parameter errors must be supplied in one of two forms as specified by the control card integer IAM.

a) Standard error form (IAM = 1). FORMAT(6F9.4)
If this input is used the covariances between the cell parameters are assumed to be zero.

Columns	
1-9	σ(a)
10-18	σ(b)
19-27	σ(c)
28-36	σ(cos α)
37-45	σ(cos β)
46-54	σ(cos γ)

b) Variance-covariance matrix form (IAM = 2). If information on the covariances between cell parameters is available, the 21 unique elements of this 6 x 6 matrix should be punched on three cards.

FORMAT(8F9.4)

Card 1: AM(a,a), AM(a,b),...., AM(a, cos γ), AM(b,b), AM(b,c).
Card 2: AM(b, cos α),...., AM(b, cos γ), AM(c,c),...., AM(cos α, cos α).
Card 3: AM(cos α, cos β),...., AM(cos γ, cos γ).

8. Symmetry cards. FORMAT(F11.6,2I2,F11.6,2I2,F11.6,2I2) The number of symmetry cards to be read is given by NS on the control card. There must be a card for each symmetry transformation which will be called for by an instruction card (see the section "Atom Designation and Symmetry Transformations"). If the functions to be computed require no symmetry transformations, then no symmetry cards need be supplied.

These symmetry cards have the same format as those for OR FLS.

Columns	
1-11	Translational part of x_j or blank.
12-13	1, 2, 3, -1, -2, -3, or blank for x, y, z, -x, -y, -z, or blank, respectively, as used in the expression for the transformed x_j.
14-15	1, 2, 3, -1, -2, -3, or blank for x, y, z, -x, -y, -z, or blank, respectively, as used in the expression for the transformed x_j. (Columns 12 and 13 are exactly equivalent to 14 and 15. Also, note that an expression such as x_j = 2x must be treated as x_j = x + x.)
16-26	Translational part of y_j or blank.
27-30	Integers representing plus or minus x, y, or z in the expression for the transformed y_j as described above.
31-41	Translational part of z_j or blank.
42-45	Integers representing plus or minus x, y, or z in the expression for the transformed z_j.

9. Instruction cards. FORMAT(24I3)
   See the next section, "Instruction Input," for the specifications for this input.

10. Instruction termination card. FORMAT(24I3)
    Columns
    1-3 0 (zero) as a sentinel for the end of the instruction deck.

INSTRUCTION INPUT

Each function to be computed by the program is specified by a sequence of integers, IN, which are read from one or more instruction cards. The first integer in this sequence, IN(1), defines the type of function to be computed, and the interpretation of the remaining instruction integers will in general be different for different types of functions. Details of the instruction integers for each type of function are given below.

Each instruction card is read with FORMAT(24I3). Of the 24 integers on this card only the first 23 are considered to be part of the instruction, IN. Usually one card will suffice to specify a function, but if a function requires more than 23 integers to define it, up to ten cards may be used with 23 integers on each card. Punching a one (or any non-zero integer) in field 24 of an instruction card indicates that the instruction is continued on the next card.

Function 1

One interatomic distance.

Columns

1-3	1	
4-6	a_1	atom designation 1.
7-9	$100c_1 + s_1$	
10-12	a_2	atom designation 2.
13-15	$100c_2 + s_2$	

Function 101

All distances (less than d(max)) between atoms in two asymmetric units.

Columns

1-3	101
4-6	a(max), the number of atoms in the parameter list.
7-9	$100c_1 + s_1$, designation of first asymmetric unit.
10-12	---
13-15	$100c_2 + s_2$, designation of second asymmetric unit. (This may be the same as the first.)
16-18	The integer 10d(max). If this is left blank, d(max) = 4.0A.

Function 201

All distances (less than d(max)) between atoms in the basic asymmetric unit and atoms in all asymmetric units (i.e., all combinations of c and s).

In order to cause this instruction to compute all possible distances less than d(max), the basic asymmetric unit should be chosen close to the origin, and the symmetry transformations specified should generate asymmetric units to fill out a unit cell on the positive sides of this basic unit. Even so, for certain symmetry situations or for small unit cells, some of the desired distances will be omitted if the atoms involved lie outside of the eight unit cells

generated. The user may prefer to use instruction 101 and to select in advance the asymmetric units likely to be involved in these contacts.

Columns

1-3	201
4-6	a(max), the number of atoms in the parameter list.
7-15	---
16-18	The integer 10d(max). If this is left blank then d(max) = 4.0A.

Function 2

Angle defined by three atoms.

Columns

1-3	2
4-9	Atom designation 1.
10-15	Atom designation 2 (vertex).
16-21	Atom designation 3.

Function 3

Angle between normals to planes each defined by three atoms. The direction of the normals is that of $(\overrightarrow{1,2})x(\overrightarrow{1,3})$ and $(\overrightarrow{4,5})x(\overrightarrow{4,6})$ where $\overrightarrow{1,2}$ is the vector defined by atom designations 1 and 2, etc.

Columns

1-3	3	
4-9	Atom designation 1	Plane 1
10-15	Atom designation 2	
16-21	Atom designation 3	
22-27	Atom designation 4	Plane 2
28-33	Atom designation 5	
34-39	Atom designation 6	

Function 4

Difference between two interatomic distances.

Columns

1-3	4	
4-9	Atom designation 1	Distance 1
10-15	Atom designation 2	
16-21	Atom designation 3	Distance 2
22-27	Atom designation 4	

Function 5

Difference between two angles each defined by three atoms.

Columns

1-3	5	
4-9	Atom designation 1	Angle 1
10-15	Atom designation 2 (vertex)	
16-21	Atom designation 3	
22-27	Atom designation 4	Angle 2
28-33	Atom designation 5 (vertex)	
34-39	Atom designation 6	

Function 6

The sum of several angles each defined by three atoms.

Columns

1-3	6	
4-6	n, the number of angles to be summed.	
7-12	Atom designation 1	Angle 1
13-18	Atom designation 2 (vertex)	
19-24	Atom designation 3	

Columns

25-30	Atom designation 4	Angle 2
31-36	Atom designation 5 (vertex)	
37-42	Atom designation 6	
	etc.	

Function 7

The RMS component of thermal displacement of one atom along principal axis r.

Columns

1-3	7
4-9	Atom designation
10-12	r (= 1, 2, or 3)

Function 107

Same as Function 7 computed for each of the three values of r.

Columns

1-3	107
4-9	Atom designation

Function 207

Same as Function 7 computed for each atom of a given asymmetric unit, each with the three values of r.

Columns

1-3	207
4-6	a(max), the number of atoms in the parameter list.
7-9	Designation of the asymmetric unit.

Function 8

Angle between principal axis r of atom 1 and a vector defined by atoms 2 and 3.

Columns

1-3	8	
4-9	Atom designation 1	
10-12	r (= 1, 2, or 3)	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	

Function 108

Same as Function 8 computed for each of the three values of r.

1-3	108	
4-9	Atom designation 1	
10-12	---	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	

Function 208

Same as Function 8 computed for each atom in a given molecule, each with the three values of r.

Columns

1-3	208	
4-6	a(max), the number of atoms in the parameter list.	
7-9	Designation of the asymmetric unit.	
10-12	---	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	

Function 9

The RMS component of thermal displacement of atom 1 along principal axis r, projected on a vector defined by atoms 2 and 3.

Columns

1-3	9	
4-9	Atom designation 1	
10-12	r (= 1, 2, or 3)	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	Vector

Function 109

Same as Function 9 computed for the three values of r.

Columns

1-3	109	
4-9	Atom designation 1	
10-12	---	
13-18	Atom designation 2	Vector
19-24	Atom designation 3	Vector

Function 209

Same as Function 9 computed for each atom in a given asymmetric unit, each with the three values of r.

Columns

1-3	209
4-6	a(max), the number of atoms in the parameter list.
7-9	Designation of the asymmetric unit.
10-12	---

Columns

13-18	Atom designation 2	Vector
19-24	Atom designation 3	

Function 10

Angle between principal axis r of atom 1 and axis i of a cartesian coordinate system. The latter is defined by atoms 2, 3, 4, and 5 as follows: Axis 1 is in the direction of vector $(\overrightarrow{2,3})$. Axis 2 is in the direction of (Axis 1)x$(\overrightarrow{4,5})$. Axis 3 is in the direction of (Axis 1)x(Axis 2).

Columns

1-3	10		
4-9	Atom designation 1		
10-12	r (= 1, 2, or 3)		
13-15	i (= 1, 2, or 3)		
16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 110

Same as Function 10 computed for the nine combinations of r and i.

Columns

1-3	110
4-9	Atom designation 1
10-15	---

Columns

16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 210

Same as Function 10 computed for all atoms in a given asymmetric unit, each with the nine combinations of r and i.

Columns

1-3	210
4-6	a(max), the number of atoms in the parameter list.
7-9	Designation of the asymmetric unit.
10-15	---

16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 11

The RMS component of thermal displacement of atom 1 along principal axis r, projected on axis i of a cartesian coordinate system defined by atoms 2, 3, 4, and 5 as described under Function 10.

Columns

1-3	11
4-9	Atom designation 1
10-12	r (= 1, 2, or 3)

Columns

13-15	i (= 1, 2, or 3)		
16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 111

Same as Function 11 computed for the nine combinations of r and i.

1-3	111		
4-9	Atom designation 1		
10-15	---		
16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 211

Same as Function 11 computed for all atoms in a given asymmetric unit, each with the nine combinations of r and i.

Columns

1-3	211
4-6	a(max), the number of atoms in the parameter list.
7-9	Designation of asymmetric unit.
10-15	---

Columns

16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 12

The RMS component of thermal displacement of atom 1 in the direction of a vector defined by atoms 2 and 3.

Columns

1-3	12	
4-9	Atom designation 1	
10-15	Atom designation 2	Vector
16-21	Atom designation 3	

Function 13

The RMS radial thermal displacement of an atom.

Columns

1-3	13
4-9	Atom designation

Function 14

Interatomic distance averaged over thermal motion. Second atom is assumed to ride on the first. The function is $\overline{R} = R_o + (\overline{r_2^2} - \overline{\xi_2^2} - \overline{r_1^2} + \overline{\xi_1^2})/2R_o$ where R_o is the uncorrected interatomic distance, $\overline{r_i^2}$ is the mean square radial thermal displacement of atom i, and $\overline{\xi_i^2}$ is the mean square component of displacement of atom i in the direction defined by the interatomic vector.

Columns

1-3	14
4-9	Atom designation 1
10-15	Atom designation 2

Function 15

Interatomic distance averaged over thermal motion. Atoms assumed to move independently. The function is $\overline{R} = R_o + (\overline{r_2^2} - \overline{\xi_2^2} + \overline{r_1^2} - \overline{\xi_1^2})/2R_o$ where the symbols are defined as in Function 14 above.

Columns

1-3	15
4-9	Atom designation 1
10-15	Atom designation 2

TAPES REQUIRED

Listed here are the monitor control cards required for operation at the Oak Ridge Central Data Processing Facility. At other installations the necessary tapes should be specified appropriately.

*TAPE(3, Reel Number, SAVE)

This tape is required only if NP = 0, indicating that information is to be taken from the output of OR FLS. It will be rewound before being read and may be file protected if desired.

*TAPE(9, OUTPUT)

This is the monitor output tape to be listed.

*TAPE(10, INPUT)

This is the monitor input tape prepared from cards.

ERROR INDICATORS

If an error is detected in the course of computing a function, an indicator is put out in place of the result, and the program proceeds to compute the next function. The form of the indicator is "***NG" where NG is an integer, the meaning of which is tabulated here.

NG	Subprogram	Meaning
1	ATOM, BETA	The symmetry position specified is out of range of the symmetry cards supplied.
4	BETA	The temperature factors are not in anisotropic form. Either ITF = 1 on OR FLS tape or JBP $<$ 6 when parameters are read from cards.
5	ATOM, BETA	The atom specified is out of range of the parameter list.
6	STOBB	A cell parameter A(1), A(2), or A(3) $\leqslant$ 0.
7	EIGVAL	The eigenvalues are complex.
8	EIGVEC	Only null eigenvectors are found.
9	COSVV	One of the vectors is null.
10	FUNXI	The vector used to specify the direction is null.
11	FUNI	The function specified is out of range. The program requires 0 $<$ XMODF(IN(1),100) $\leqslant$ 15.

SPECIFICATIONS FOR SUBROUTINES TO COMPUTE NEW TYPES OF FUNCTIONS

To program a new type of function the user selects a function designation integer, i. Function designations 1-15 have already been assigned in the program as written so that normally new designations would be 16, 17....

Subprograms HEDI, PREI, FUNI, and OUTI must each be modified as follows:

1. Change the second IF statement to permit the new function designation.
2. Add a branch to the computed GO TO.
3. Add a CALL statement for the new routine followed by a GO TO 160.

The user then writes four Fortran II subroutines named HEDi, PREi, FUNi, and OUTi as described below. All these subprograms are compiled and added to the binary deck removing the original routines where necessary.

The programmer should refer to the symbolic listing of functions 1-15 for examples of the following routines.

HEDi

The user may omit this subroutine if desired. Its purpose is to put out an over-all heading which defines the type of function. It is entered each time the function designation IN(1) is changed.

1. The subroutine has no arguments.
2. No COMMON or DIMENSION statements are needed.
3. Put out the heading on tape 9.
4. The first Hollerith character should be zero to cause double spacing.
5. More than one line may be put out if desired.

PREi

This subroutine need be included only if standard errors are to be computed. Its purpose is to instruct the program as

to which parameters are involved in the function to be computed. The program thus avoids computing unnecessary derivatives.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout the program.
3. Enter the subroutines SETKX and/or SETKB once for each atom involved in the function. See the section "Arithmetic Subprograms Available" for details of these routines.

FUNi

The purpose of this subroutine is to compute the desired function when given the various input data found in common storage.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout the program.
3. The significance of the instruction integers IN(K) except for IN(1) is at the discretion of the programmer.
4. The necessary atomic coordinates or temperature factor coefficients are called for by means of subroutines ATOM or BETA.
5. If the metric tensors AA or BB are to be used, the subroutines STOAA and/or STOBB must be entered. See the section "Arithmetic Subprograms Available" for a description of these routines.

6. Store the function at FX in COMMON and RETURN.

OUTi

The purpose of this subroutine is to put out the detailed description of the individual function computed. Its inclusion is optional but certainly desirable.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout Segment 2.
3. The description which probably includes the relevant instruction integers, IN, should be put out on tape 9.
4. The first character of the first line of this description should be a Hollerith zero to cause double spacing.
5. More than one line may be put out if desired.

ARITHMETIC SUBPROGRAMS AVAILABLE

1. CALL SETKX (IN(K))

Instructs the program to calculate derivatives with respect to the coordinates of the atom designated in IN(K). This subroutine is used by the preliminary subroutines, PREi.

2. CALL SETKB (IN(K))

Instructs the program to calculate derivatives with respect to the anisotropic temperature factor coefficients of the atom designated in IN(K). This subroutine is used by the preliminary subroutines, PREi.

3. CALL STOAA

Stores the 3 x 3 metric tensor $\underset{\sim}{g}$ (where $g_{ij} = \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j$) at AA in common storage.

4. CALL STOBB

Stores the 3 x 3 reciprocal metric tensor $\underset{\sim}{g}^{-1}$ (where $(g^{-1})_{ij} = \underset{\sim}{b}_i \cdot \underset{\sim}{b}_j$) at BB in common storage.

5. CALL ATOM(IN(K),Z)

DIMENSION Z(3)

Stores at Z the coordinates of the atom specified by the instruction integers IN(K) and IN(K+1). These coordinates refer to the triclinic axes. They have been transformed according to the symmetry specified.

6. CALL BETA (IN(K),Z)

DIMENSION Z(3,3)

Stores at Z the 3 x 3 matrix of the temperature factor coefficients of the atom specified by instruction integers IN(K) and IN(K+1). The matrix has been transformed according to the symmetry specified.

7. CALL MM (X, Y, Z)

DIMENSION X(3,3), Y(3,3), Z(3,3)

Performs the matrix multiplication $\underset{\sim}{X}\underset{\sim}{Y} = \underset{\sim}{Z}$. The location of $\underset{\sim}{Z}$ must be different from $\underset{\sim}{X}$ and $\underset{\sim}{Y}$.

8. CALL MV (X, Y, Z)

DIMENSION X(3,3), Y(3), Z(3)

Performs the matrix-vector multiplication $\underset{\sim}{X}\underset{\sim}{Y} = \underset{\sim}{Z}$. The location of $\underset{\sim}{Z}$ must be different from $\underset{\sim}{Y}$.

9. CALL VM (X, Y, Z)

DIMENSION X(3), Y(3,3), Z(3)

Performs the vector-matrix multiplication $\underset{\sim}{X}^T\underset{\sim}{Y} = \underset{\sim}{Z}^T$. The locations of $\underset{\sim}{Z}$ must be different from $\underset{\sim}{X}$.

10. Function VV(X, Y)

DIMENSION X(3), Y(3)

Performs the vector-vector multiplication $\underset{\sim}{X}^T\underset{\sim}{Y} = Z$ (a scalar).

11. Function VMV (W, X, Y)

DIMENSION W(3), X(3,3), Y(3)

Performs the vector-matrix-vector multiplication $\underset{\sim}{W}^T\underset{\sim}{X}\underset{\sim}{Y} = \underset{\sim}{Z}$ (a scalar).

12. CALL DIFV (X, Y, Z)

DIMENSION X(3), Y(3), Z(3)

Performs the vector subtraction $\underset{\sim}{X} - \underset{\sim}{Y} = \underset{\sim}{Z}$. $\underset{\sim}{Z}$ may have the same location as $\underset{\sim}{X}$ or $\underset{\sim}{Y}$.

13. CALL SUMV (X, Y, Z)

DIMENSION X(3), Y(3), Z(3)

Performs the vector summation $\underset{\sim}{X} + \underset{\sim}{Y} = \underset{\sim}{Z}$. $\underset{\sim}{Z}$ may have the same location as $\underset{\sim}{X}$ or $\underset{\sim}{Y}$.

14. Function COSVV (X, Y)

DIMENSION X(3), Y(3)

Computes the cosine of the angle defined by vectors $\underset{\sim}{X}$ and $\underset{\sim}{Y}$. These vectors are assumed to refer to the triclinic coordinate system, and it is also assumed that the metric tensor has been stored at AA in common storage.

15. Function ARCCOS (X)

Computes θ, the arc cos of X in degrees. $0 \leqslant \theta \leqslant 180$.

16. CALL NORM (X, Y, Z)

DIMENSION X(3), Y(3), Z(3)

Stores at $\underset{\sim}{Z}$ a vector (not a unit vector) perpendicular to both $\underset{\sim}{X}$ and $\underset{\sim}{Y}$. The sense of $\underset{\sim}{Z}$ is that of the vector product $\underset{\sim}{X} \times \underset{\sim}{Y}$. All vectors are referred to the triclinic coordinate system, and it is assumed that the reciprocal metric tensor has been stored at BB in common storage.

17. CALL AXES (U, V, X)

DIMENSION U(3), V(3), X(3,3)

Stores three mutually perpendicular vectors (not unit vectors) at X(I,1), X(I,2), and X(I,3). X(I,1) = U(I). X(I,2) is normal to $\underset{\sim}{U}$ and $\underset{\sim}{V}$, i.e., in the direction of $\underset{\sim}{U} \times \underset{\sim}{V}$. X(I,3) is normal to X(I,1) and X(I,2) so as to yield a right-handed coordinate system. All these vectors are referred to the triclinic coordinate system, and it is assumed that the reciprocal metric tensor has been stored at BB in common storage.

18. CALL EIGVAL (W, Y)

DIMENSION W(3,3), Y(3)

Stores the three eigenvalues Y of the matrix $\underset{\sim}{W}$.

The method used for solving the cubic determinental equation is that described by R. S. Burington, Handbook of Mathematical Tables and Formulas, (Handbook Publishers, Inc., Sandusky, Ohio, 1956), 3rd ed., pp. 7-9.

19. CALL EIGVEC (W, Y, Z)

DIMENSION W(3,3), Z(3)

Given an eigenvalue Y of the matrix W, this subroutine stores the corresponding eigenvector Z.

Solving any pair of the three available equations would yield a vector in the desired direction. Because of special symmetry situations, however, the pairs chosen could be redundant so that a null vector would be obtained. The subroutine therefore repeats the calculation with each of the three possible pairs, and the vector of largest magnitude is taken as the correct result. If all three pairs yield null vectors, the subroutine sets an error indicator, because this implies that the direction of the eigenvector is indeterminate.

20. Function TRACE (X)

DIMENSION X(3,3)

Computes the trace of the matrix X.

DISCUSSION OF EXAMPLES

Data for two test problems are included with the card deck for OR FFE. Both are extensions of the hypothetical problem based on alpha quartz which was included with the program OR FLS. Example 1 uses card input only, and tests the present program independently. Example 2 takes part of its input from a tape produced by OR FLS, and tests the two programs together. To obtain the required magnetic tape from OR FLS it is necessary to modify the test data card FLS 1414 by substituting 1 for 0 in column 18.

It should be emphasized again that this problem is a hypothetical one. Although the structure considered is qualitatively that of alpha quartz, the observations used in the OR FLS test are synthetic, and the parameters which result are not related to the true structure of this material.

Silicon atom (2,300) lies on a single twofold rotation axis and has oxygen atoms (1,2), (1,3), (1,300), and (1,305) as four nearest neighbors in an approximately tetrahedral configuration. Example 1 computes the independent distances and angles of this group. The dihedral angle computed is a measure of the distortion of the tetrahedron. The differences computed show how the program can be used to determine whether chemically equivalent but crystallographically distinct distances or angles have significant deviations from each other.

Example 2 includes computations relating to the anisotropic temperature factor coefficients. First the root-mean-square displacements in the principal axis directions are obtained. Then the angles which principal axes of the O atom (1,2) make with the Si-O bond (2,300) (1,2) are computed. Next a cartesian coordinate system is defined in terms of the Si-O vectors (2,300) (1,2) and (2,300) (1,3) so that the principal axes of O can be related to this. Note that the axis with I = 1 is just the Si-O bond direction used above so that the angles with I = 1 repeat those computed earlier.

Because the Si atom is located on a twofold axis, one of its principal axes is constrained to lie in that direction.

By choosing a coordinate system based on Si atoms in different cells, cartesian axis 1 is made to fall on the twofold axis, axis 2 lies in the x,y plane and axis 3 is parallel to z. Principal axes 1 and 3 are both seen to make angles of 90° with cartesian axis 1, as expected. Principal axis 2 should therefore make angles of 0° (or 180°), 90°, and 90° with cartesian axes 1, 2, and 3, respectively. Unfortunately, the results are only approximately correct in the present test problem. The parameters from the hypothetical OR FLS test problem represent atoms which are nearly isotropic, and it is believed that this situation permits round-off errors to cause the observed discrepancies.

Finally three other types of functions are computed to complete the test.

CARD DECKS PROVIDED†

Subprogram	Symbolic card numbers	Column binary card numbers*
Calling program	1 - 246	2051 - 2103**
SUB8	247 - 300	2104 - 2109
SUB10	301 - 321	2110 - 2112
SUB11	322 - 347	2113 - 2115
SUB13	348 - 491	2116 - 2133
SUB19	492 - 508	2134 - 2136
SUB21	509 - 581	2137 - 2145
HEDI	582 - 637	2146 - 2155

Subprogram	Symbolic card numbers	Column binary card numbers*
PREI	638 - 678	2156 - 2162
FUNI	679 - 746	2163 - 2172
OUTI	747 - 786	2173 - 2179
SETKX	787 - 803	2180 - 2182
SETKB	804 - 820	2183 - 2186
STOAA	821 - 840	2187 - 2190
STOBB	841 - 874	2191 - 2197
ATOM	875 - 927	2198 - 2209
BETA	928 - 987	2210 - 2224
MM	988 - 999	2225 - 2228
MV	1000 - 1010	2229 - 2232
VM	1011 - 1021	2233 - 2236
VV	1022 - 1031	2237 - 2239
VMV	1032 - 1040	2240 - 2242
DIFV	1041 - 1049	2243 - 2245
SUMV	1050 - 1058	2246 - 2248
COSVV	1059 - 1075	2249 - 2253
ARCCOS	1076 - 1081	2254 - 2256
NORM	1082 - 1101	2257 - 2260
AXES	1102 - 1113	2261 - 2265
EIGVAL	1114 - 1160	2266 - 2277
EIGVEC	1161 - 1195	2278 - 2284
TRACE	1196 - 1204	2285 - 2287
FUNA	1205 - 1224	2288 - 2292

Subprogram	Symbolic card numbers	Column binary card numbers*
FUND	1225 - 1241	2293 - 2296
HED1	1242 - 1248	2297 - 2299
PRE1	1249 - 1261	2300 - 2302
FUN1	1262 - 1273	2303 - 2305
OUT1	1274 - 1286	2306 - 2308
HED2	1287 - 1293	2309 - 2311
PRE2	1294 - 1306	2312 - 2314
FUN2	1307 - 1318	2315 - 2317
OUT2	1319 - 1331	2318 - 2320
HED3	1332 - 1339	2321 - 2323
PRE3	1340 - 1352	2324 - 2326
FUN3	1353 - 1377	2327 - 2333
OUT3	1378 - 1391	2334 - 2337
HED4	1392 - 1398	2338 - 2340
PRE4	1399 - 1411	2341 - 2343
FUN4	1412 - 1423	2344 - 2346
OUT4	1424 - 1437	2347 - 2350
HED5	1438 - 1444	2351 - 2353
FUN5	1445 - 1456	2354 - 2356
HED6	1457 - 1463	2357 - 2359
PRE6	1464 - 1477	2360 - 2362
FUN6	1478 - 1492	2363 - 2365
OUT6	1493 - 1507	2366 - 2369
FUNB	1508 - 1527	2370 - 2374

Subprogram	Symbolic card numbers	Column binary card numbers*
FUNC	1528 - 1548	2375 - 2379
FUNX	1549 - 1573	2380 - 2386
HED7	1574 - 1581	2387 - 2390
PRE7	1582 - 1593	2391 - 2393
FUN7	1594 - 1606	2394 - 2396
OUT7	1607 - 1619	2397 - 2399
HED8	1620 - 1627	2400 - 2403
PRE8	1628 - 1641	2404 - 2406
FUN8	1642 - 1654	2407 - 2409
OUT8	1655 - 1668	2410 - 2413
HED9	1669 - 1677	2414 - 2417
FUN9	1678 - 1690	2418 - 2420
HED10	1691 - 1699	2421 - 2424
PRE10	1700 - 1713	2425 - 2427
FUN10	1714 - 1726	2428 - 2430
OUT10	1727 - 1741	2431 - 2434
HED11	1742 - 1751	2435 - 2438
FUN11	1752 - 1764	2439 - 2441
FUNR	1765 - 1780	2442 - 2445
FUNCR	1781 - 1799	2446 - 2451
FUNXI	1800 - 1824	2452 - 2457
HED12	1825 - 1833	2458 - 2461
PRE12	1834 - 1847	2462 - 2464
FUN12	1848 - 1860	2465 - 2467

Subprogram	Symbolic card numbers	Column binary card numbers*
OUT12	1861 - 1874	2468 - 2471
HED13	1875 - 1881	2472 - 2474
FUN13	1882 - 1894	2475 - 2477
OUT13	1895 - 1907	2478 - 2480
HED14	1908 - 1915	2481 - 2483
PRE14	1916 - 1929	2484 - 2486
FUN14	1930 - 1943	2487 - 2489
HED15	1944 - 1951	2490 - 2492
FUN15	1952 - 1965	2493 - 2495
ASIN		2496 - 2499***
SETA (Dummy)	1966 - 1970	2500 - 2501
SETP (Dummy)	1971 - 1975	2502 - 2503
SETA (Examples 1 and 2)	1976 - 1982	2504 - 2506
SETP (Example 1)	1983 - 1989	2507 - 2509
SETP (Example 2)	1990 - 1998	2510 - 2512
Transfer card and data for Example 1	1999 - 2022	
Transfer card and data for Example 2	2023 - 2050	

*The column binary cards provided were compiled on an IBM 7090. Most of the subprograms must be recompiled if they are to be used on an IBM 704.

**Card No. 2051 is a control card for the Oak Ridge monitor system. It may not be appropriate at other installations.

***The ASIN routine is included because it is not available from the Oak Ridge library tape. It may not be needed at other installations. Library routines SQRT, COS, and EXIT (which terminates the job) should also be inserted here if they are not supplied by the monitor system.

†Users who received a temporary card deck during 1963 will probably find that the only change has been to add identifying numbers to the final version. The most recent modifications to the program were made in the cards now numbered FFE 072, 073, 162, 939, 940, and 1140-1143. If these cards are verified and corrected where necessary, then the temporary deck will conform to this report.

GLOSSARY OF SYMBOLS

The following list defines the symbols used in the main parts of the program. Some of the independent arithmetic subroutines repeat certain symbols with different meanings, and these are not included in this glossary.

Arrays are represented by symbols followed by their minimum allowable dimensions. All other symbols refer to single-storage variables. Those marked with an asterisk (*) are sometimes read as input data.

*A(6)	Direct cell parameters a, b, c, cos α, cos β, and cos γ.
AA(3,3)	Metric tensor $\underset{\sim}{g}$ where $g_{ij} = \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j$.
AM(21)	Upper triangular part of the variance-covariance matrix associated with the six cell parameters. AM(1) = U_{11}, AM(2) = U_{12},..., AM(6) = U_{16}, AM(7) = U_{22},...., etc.
BB(3,3)	Reciprocal metric tensor $\underset{\sim}{g}^{-1}$ where $(g^{-1})_{ij} = \underset{\sim}{b}_i \cdot \underset{\sim}{b}_j$.
C	Factor C_{ij} used in computing variances in SUB13. $C_{ij} = 1$ if $i = j$; otherwise $C_{ij} = 2$.
DA(6)	Increments $\Delta a_i = (0.01)\ U_{ii}^{1/2}$.
DFDA(6)	Derivatives $\partial f/\partial a_i$.
DFDP(NV)	Derivatives $\partial f/\partial p_i$.
DMAX	Maximum distance which will be printed when using instructions 101 or 201.
DP(NV)	Increments $\Delta p_i = (0.01)\ V_{ii}^{1/2}$.
E	Standard error, e, of the function including contributions from cell parameter errors and atomic parameter errors.

E1	Standard error, e′, of the function including only contributions from least-squares parameter errors.
F	Computed value of function f to be put out.
FX	Computed value of function f as stored by the subroutines FUNi.
*IAM	Cell parameter error indicator. If IAM = 0, cell parameter errors are not to be used. If IAM = 1, they are to be read as standard errors. If IAM = 2, they are to be read as a variance-covariance matrix.
IH	Hundreds digit of the instruction number, IN(1).
*IN(231)	Array of integers used to define the function to be computed. IN(1) specifies the kind of function.
INSAVE	IN(1) saved from the previous instruction integers. The function heading is put out if IN(1) ≠ INSAVE.
*IPM	Atomic parameter error indicator. If IPM = 0, these errors will not be used in computing the standard error of the function. If IPM = 1, they will be used.
*IS(2,3,NS)	Integers representing the non-translational part of the symmetry information. For example, if the Jth symmetry transformation is y-x, -x, 1/3 + z, this information would be stored as follows:

```
TS(1,J)   = 0.0
IS(1,1,J) = 2 (for y)
IS(2,1,J) = -1 (for -x)
TS(2,J)   = 0.0
IS(1,2,J) = -1 (for -x)
IS(2,2,J) = 0
TS(3,J)   = 0.333333
IS(1,3,J) = 3 (for z)
IS(2,3,J) = 0
```

ITF	Temperature factor indicator. ITF = 0 if parameters were read from cards. Otherwise ITF is read from the private output tape of OR FLS and is 1 or 2 for isotropic or anisotropic temperature factors, respectively.

*JB	Position of the first temperature factor coefficient in the parameter list.
*JBP	Period of the temperature factor coefficients in the parameter list.
*JX	Position of the first x-coordinate in the parameter list.
*JXP	Period of the coordinates in the parameter list.
*KI1(NP)	Parameter selection integers. KI1(I) = 1 if P(I) corresponds to a row-column of the variance-covariance matrix, PM. Otherwise KI1(I) = 0.
KI2(NP)	Integers set by subroutine PREi to specify the parameters involved in the function being computed. KI2(I) is set to 1 if P(I) is involved in the function. Otherwise KI2(I) = 0.
KK	Index used so that PM(KK) is a diagonal element of the variance-covariance matrix.
KKD	Increment to be added to KK to step from one diagonal element of PM to the next.
LNZ	Integer saved to record that DFDP(LNZ) is the last non-zero derivative in the array.
NA	Number of atoms in the parameter list as specified by the instruction integers for certain multivalued functions.
NG	Error indicator set to a non-zero integer when an error is found in the course of calculating a function or its derivative. See the section "Error Indicators" for a list of these errors.
NM	NV(NV+1)/2, the number of elements in the upper triangular part of the variance-covariance matrix, PM.
*NP	Number of parameters in the parameter list.
NQ	Number of scale factors in a parameter list which has been read from the private output tape of OR FLS.

*NS	Number of symmetry cards read.
NSP	NS+1, the number of symmetry positions including the basic asymmetric unit.
*NV	Order of the variance-covariance matrix for the atomic parameters.
*P(NP)	List of atomic parameters read either from cards or from the private output tape of OR FLS.
*PM(NM)	Upper triangular part of variance-covariance matrix associated with the atomic parameters PM(1) = V_{11}, PM(2) = V_{12}, ..., PM(NV) = $V_{1,NV}$, PM(NV+1) = V_{22}, ..., etc.
ROW(6)	Auxiliary array used in putting out the matrix AM.
SAVEA	Temporary storage for a cell parameter which is being incremented during the derivative calculation.
SAVEP	Temporary storage for an atomic parameter which is being incremented during the derivative calculation.
*SCALE	Constant used to scale the variance-covariance matrix if it is read from cards.
*TITLE(12)	Alphanumeric title read at the start of the problem and transcribed to the output.
*TS(3,NS)	Translational part of symmetry information. (See IS for an example.)
VARA	Variance of f based on the cell parameter errors only.
VARP	Variance of f based on the atomic parameter errors only.

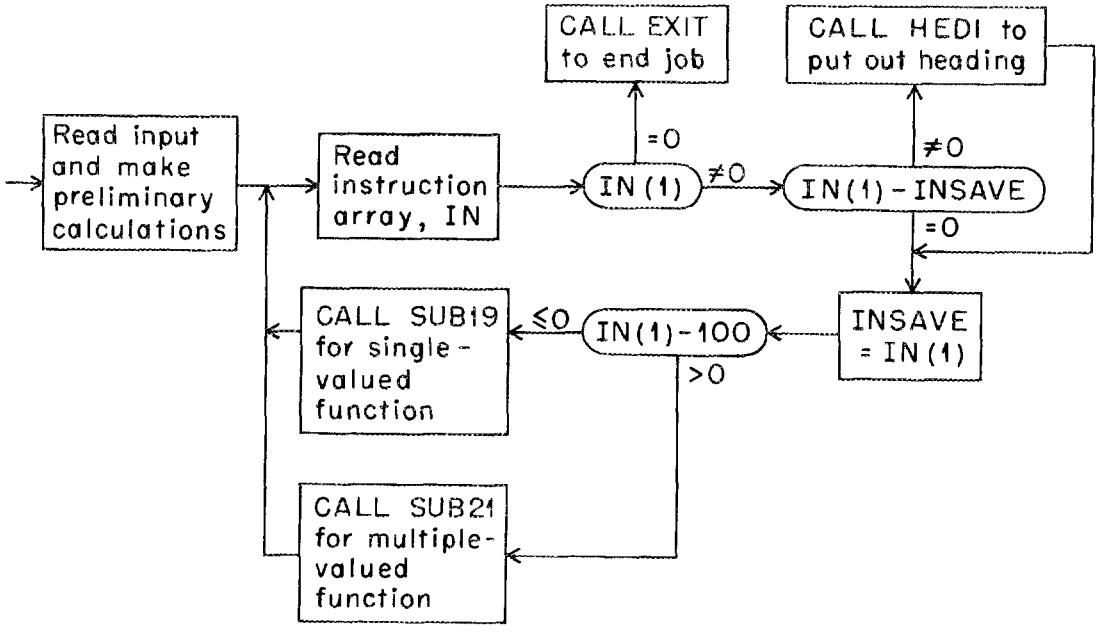

Figure 1. Schematic flow diagram of the main program showing the subprograms called by it.

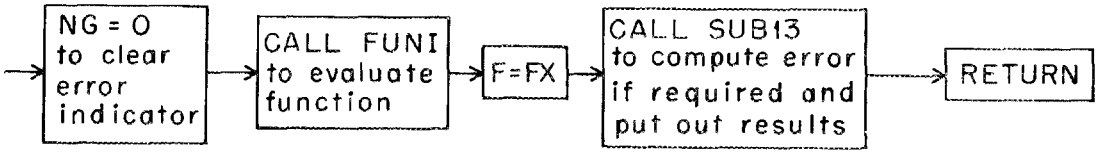

Figure 2. SUB19 which controls the calculation and output for a single-valued function.

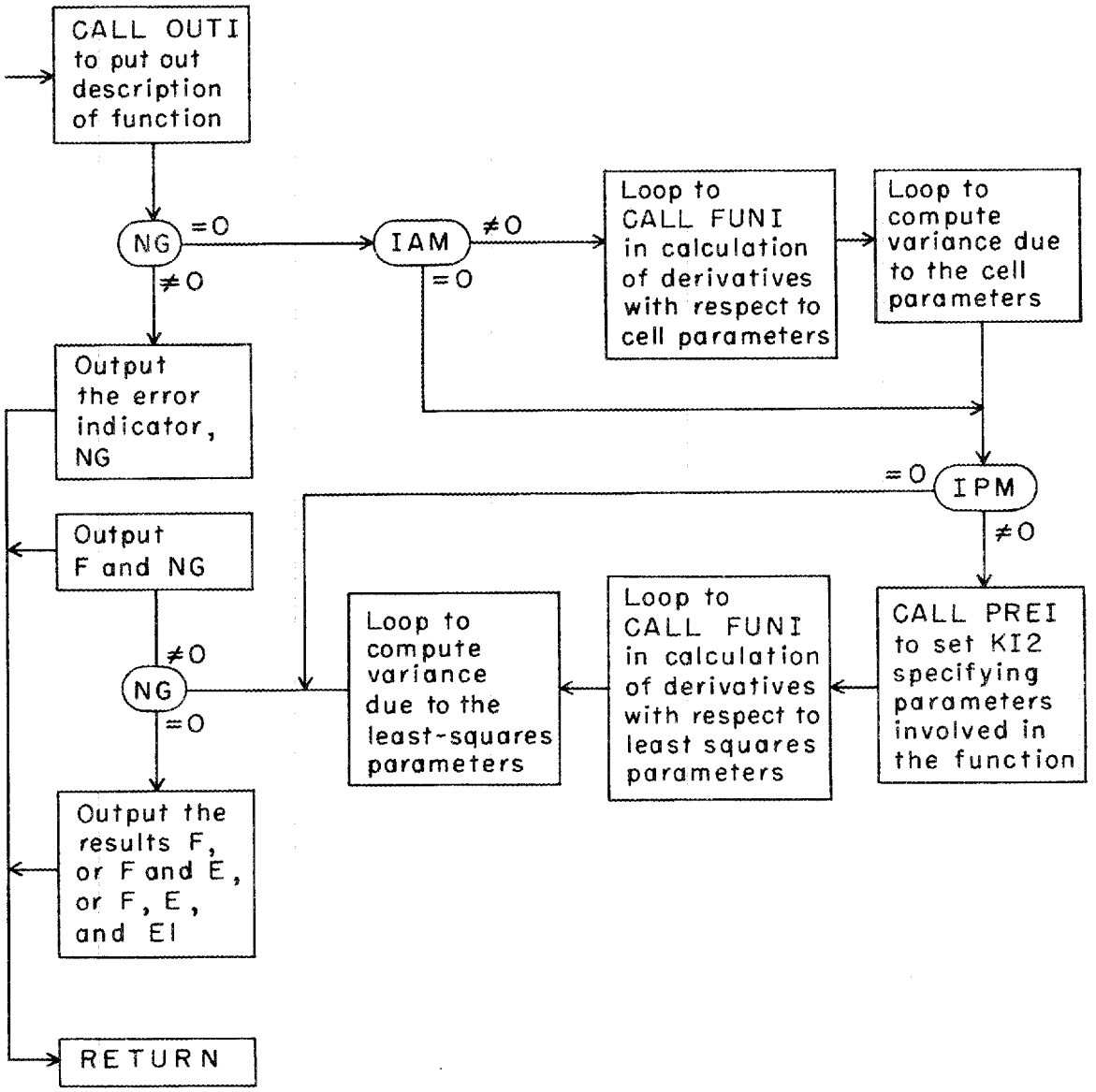

Figure 3. SUB13 which calculates the error if required and puts out the results.

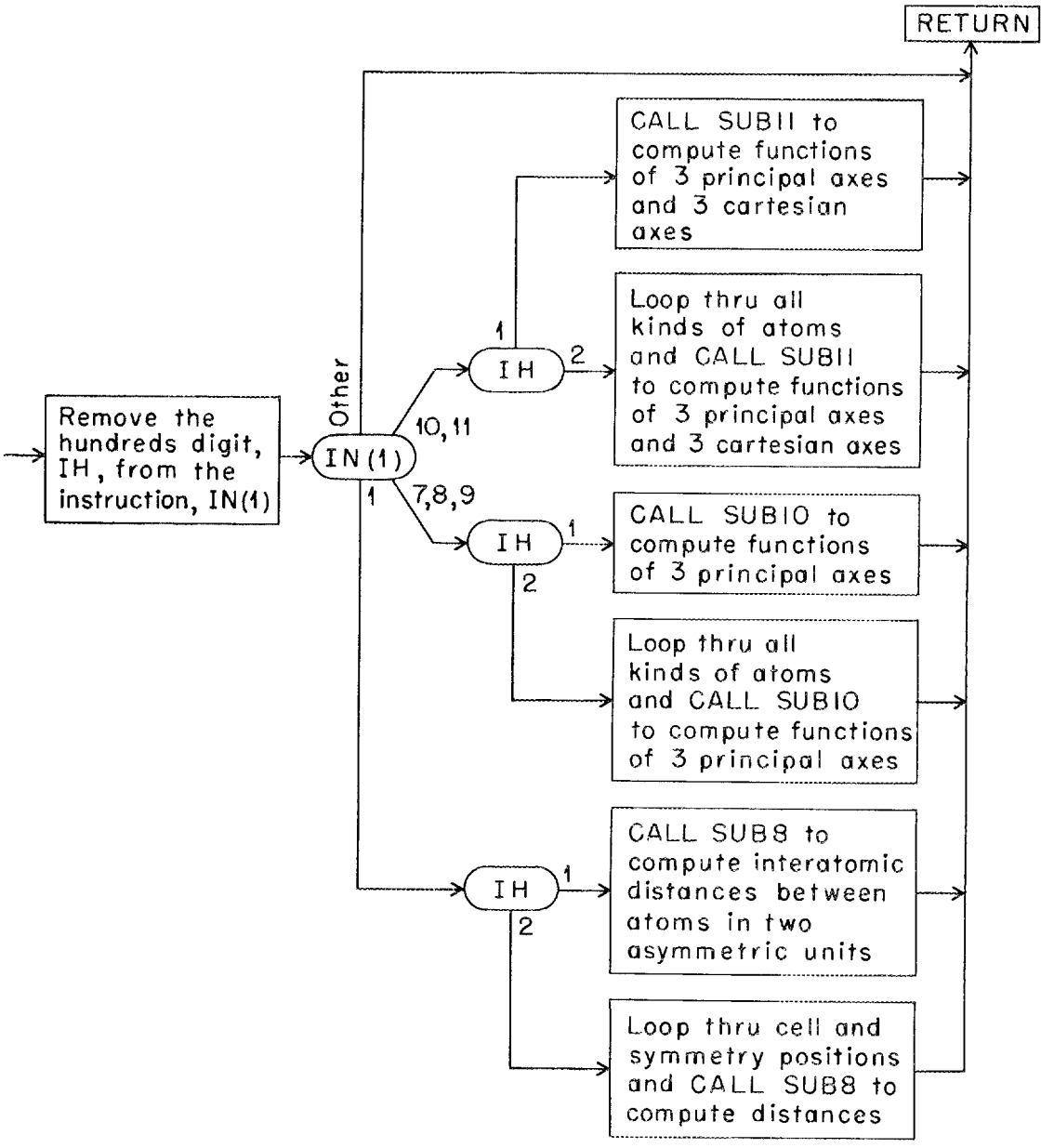

Figure 4. SUB21 which controls the calculations for multiple-values functions.

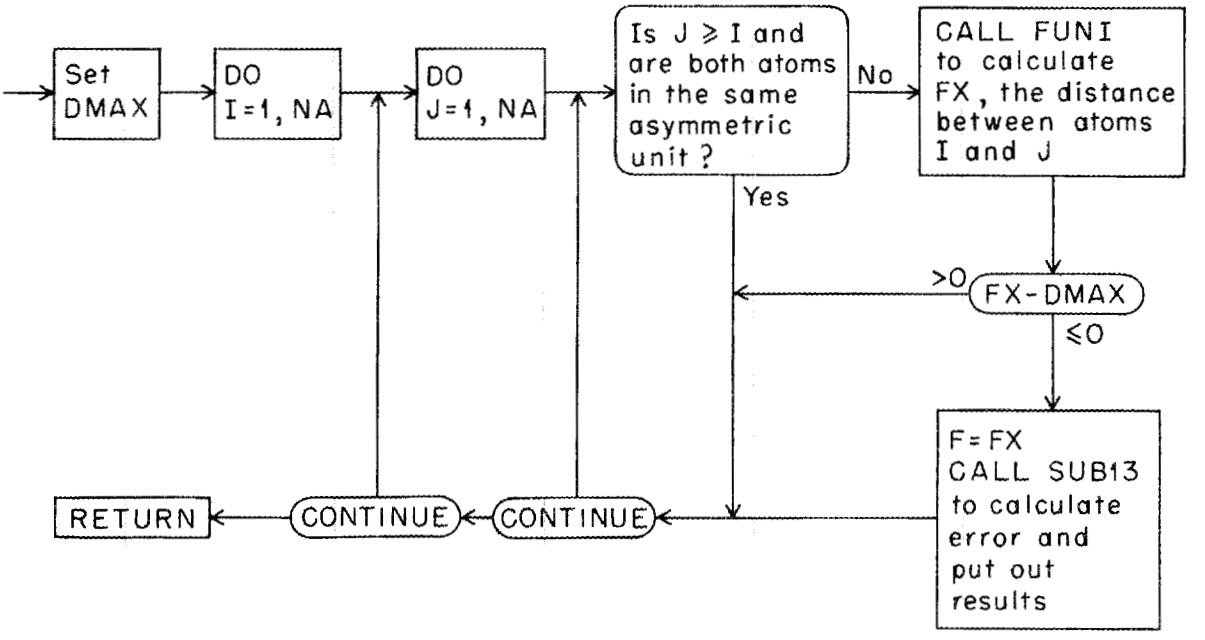

Figure 5. SUB8 which calculates all distances less than DMAX between atoms of two asymmetric units.

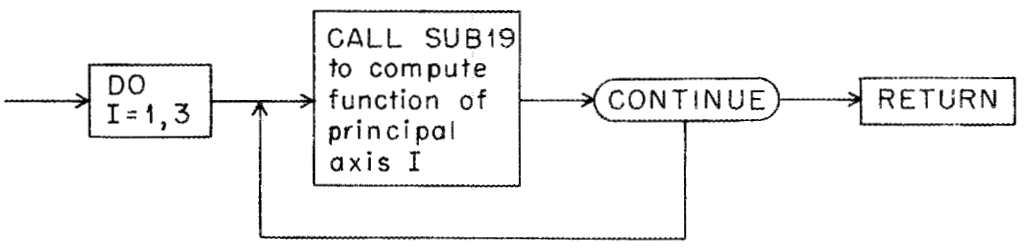

Figure 6. SUB10 which controls the calculation of funtions of each of the three principal axes of thermal motion.

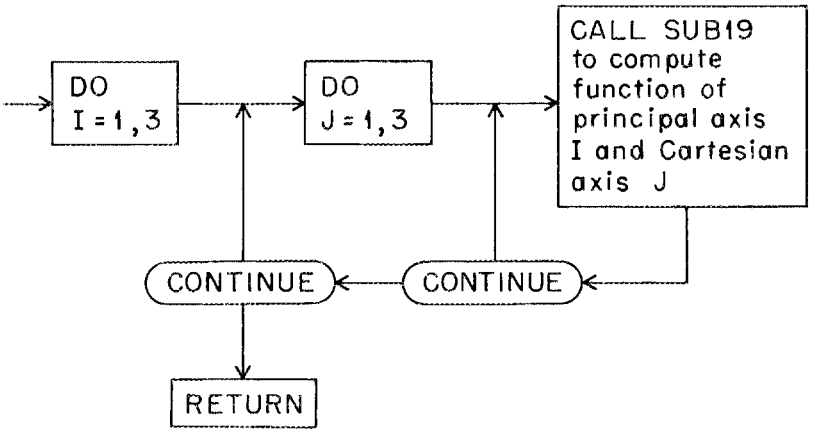

Figure 7. SUB11 which controls the calculation of functions of each of the three principal axes and of three axes of a specified cartesian coordinate system.

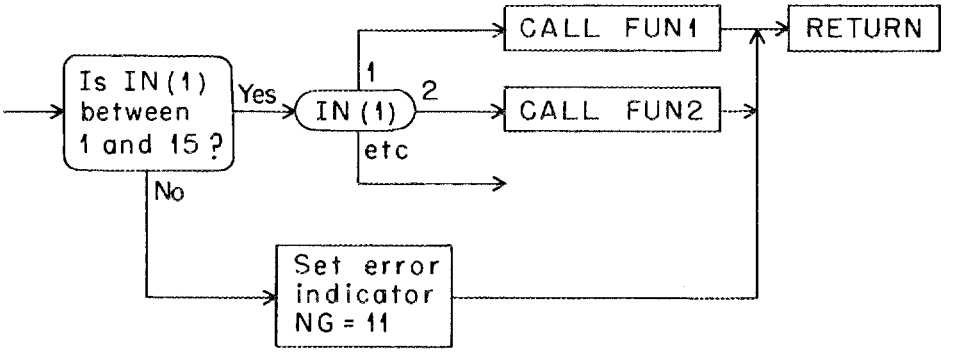

Figure 8. FUNI which transfers control to the appropriate function-calculating subroutine. HEDI, PREI, and OUTI are almost analogous to FUNI.

SYMBOLIC PROGRAM LISTING

```
*TYPE(FORTRAN)                                                          FFE  001
C     OR FFE. FORTRAN CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM       FFE  002
C     CALLING PROGRAM                                                   FFE  003
                                                                        FFE  004
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  005
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  006
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  007
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  008
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  009
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  010
                                                                        FFE  011
C     READ AND PUT OUT TITLE AND CONTROL CARD                           FFE  012
      READ INPUT TAPE 10,00102,(TITLE(I),I#1,12)                        FFE  013
00102 FORMAT (12A6)                                                     FFE  014
      WRITE OUTPUT TAPE 9,00104,(TITLE(I),I#1,12)                       FFE  015
00104 FORMAT (1H112A6)                                                  FFE  016
      READ INPUT TAPE 10,00202,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB           FFE  017
00202 FORMAT (24I3)                                                     FFE  018
      IF(NP)00297,00294,00297                                           FFE  019
                                                                        FFE  020
00294    WRITE OUTPUT TAPE 9,00295                                      FFE  021
00295    FORMAT (39H0INPUT DATA TO BE READ FROM OR FLS TAPE)            FFE  022
         GO TO 00301                                                    FFE  023
                                                                        FFE  024
00297    WRITE OUTPUT TAPE 9,00298,NP                                   FFE  025
00298    FORMAT (33H0INPUT DATA TO BE READ FROM CARDS/                  FFE  026
     1      34H0NUMBER OF STRUCTURE PARAMETERS ISI4)                    FFE  027
                                                                        FFE  028
00301 WRITE OUTPUT TAPE 9,00302                                         FFE  029
00302 FORMAT (68H0VARIANCE-COVARIANCE MATRIX AND PARAMETER SELECTION INFFFE  030
     1ORMATION WILL)                                                    FFE  031
      IF(IPM)00308,00305,00308                                          FFE  032
                                                                        FFE  033
00305    WRITE OUTPUT TAPE 9,00306                                      FFE  034
00306    FORMAT (12H NOT BE USED)                                       FFE  035
         GO TO 00310                                                    FFE  036
                                                                        FFE  037
00308    WRITE OUTPUT TAPE 9,00309                                      FFE  038
00309    FORMAT (8H BE USED)                                            FFE  039
                                                                        FFE  040
00310 WRITE OUTPUT TAPE 9,00311,NS                                      FFE  041
00311 FORMAT (28H0NUMBER OF SYMMETRY CARDS ISI3)                        FFE  042
      WRITE OUTPUT TAPE 9,00314                                         FFE  043
00314 FORMAT (26H0CELL PARAMETER ERRORS ARE)                            FFE  044
      IF(IAM-1)00316,00319,00322                                        FFE  045
                                                                        FFE  046
00316    WRITE OUTPUT TAPE 9,00317                                      FFE  047
00317    FORMAT (15H NOT TO BE USED)                                    FFE  048
         GO TO 00401                                                    FFE  049
                                                                        FFE  050
00319    WRITE OUTPUT TAPE 9,00320                                      FFE  051
00320    FORMAT (42H TO BE READ IN THE FORM OF STANDARD ERRORS)         FFE  052
         GO TO 00401                                                    FFE  053
                                                                        FFE  054
00322    WRITE OUTPUT TAPE 9,00323                                      FFE  055
00323    FORMAT (48H TO BE READ IN THE FORM OF A VARIANCE-COVARIANCE    FFE  056
     1      7H MATRIX)                                                  FFE  057
                                                                        FFE  058
00401 IF(NP)01001,01001,00501                                           FFE  059
                                                                        FFE  060
C        READ PARAMETERS AND VARIANCE-COVARIANCE MATRIX FROM CARDS      FFE  061
00501    WRITE OUTPUT TAPE 9,00502,NV                                   FFE  062
00502    FORMAT (44H0ORDER OF THE VARIANCE-COVARIANCE MATRIX FOR        FFE  063
     1      28H THE STRUCTURE PARAMETERS ISI3)                          FFE  064
         IF(JXP)00509,00509,00505                                       FFE  065
                                                                        FFE  066
```

```
00505        WRITE OUTPUT TAPE 9,00506,JXP,JX                                FFE  067
00506        FORMAT (41H0PERIOD OF THE POSITION PARAMETERS IN THE            FFE  068
     1          18H PARAMETER LIST ISI3/22H0POSITION OF THE FIRST            FFE  069
     2          38H X COORDINATE IN THE PARAMETER LIST ISI3)                 FFE  070
                                                                             FFE  071
00509     ITF#0                                                              FFE  072
          IF(JBP)00601,00601,00510                                           FFE  073
                                                                             FFE  074
00510        WRITE OUTPUT TAPE 9,00511,JBP,JB                                FFE  075
00511        FORMAT (46H0PERIOD OF THE TEMPERATURE FACTOR COEFFICIENTS       FFE  076
     1          25H IN THE PARAMETER LIST ISI3/16H0POSITION OF THE           FFE  077
     2          44H FIRST TEMPERATURE FACTOR COEFFICIENT IN THE              FFE  078
     3          18H PARAMETER LIST ISI3)                                     FFE  079
                                                                             FFE  080
00601     READ INPUT TAPE 10,00603,(P(I),I#1,NP)                             FFE  081
00603     FORMAT (8F9.4)                                                     FFE  082
          IF(IPM)00801,02101,00801                                           FFE  083
                                                                             FFE  084
00801        READ INPUT TAPE 10,00802,(KII(I),I#1,NP)                        FFE  085
00802        FORMAT (72I1)                                                   FFE  086
             NM#(NV*(NV+1))/2                                                FFE  087
             READ INPUT TAPE 10,00905,SCALE                                  FFE  088
             READ INPUT TAPE 10,00905,(PM(I),I#1,NM)                         FFE  089
00905        FORMAT (6E12.6)                                                 FFE  090
             DO 00952 I#1,NM                                                 FFE  091
                                                                             FFE  092
00952           PM(I)#PM(I)*SCALE                                            FFE  093
                                                                             FFE  094
             GO TO 02101                                                     FFE  095
                                                                             FFE  096
C         READ PARAMETERS AND VARIANCE-COVARIANCE MATRIX                     FFE  097
C                                                FROM OR FLS TAPE            FFE  098
01001     REWIND 3                                                           FFE  099
          READ INPUT TAPE 3,00202,ITF,NQ,NP                                  FFE  100
          WRITE OUTPUT TAPE 9,01004,NP                                       FFE  101
01004     FORMAT (34H0NUMBER OF STRUCTURE PARAMETERS ISI4)                   FFE  102
          READ INPUT TAPE 3,01007,(P(I),I#1,NP)                              FFE  103
01007     FORMAT (10F12.8)                                                   FFE  104
          JX#NQ+4                                                            FFE  105
          JB#NQ+7                                                            FFE  106
          IF(ITF-1)01301,01301,01401                                         FFE  107
                                                                             FFE  108
01301        JXP#6                                                           FFE  109
             JBP#6                                                           FFE  110
             GO TO 01501                                                     FFE  111
                                                                             FFE  112
01401        JXP#11                                                          FFE  113
             JBP#11                                                          FFE  114
                                                                             FFE  115
01501     WRITE OUTPUT TAPE 9,00506,JXP,JX                                   FFE  116
          WRITE OUTPUT TAPE 9,00511,JBP,JB                                   FFE  117
          IF(IPM)01701,02101,01701                                           FFE  118
                                                                             FFE  119
01701        READ INPUT TAPE 3,00802,(KII(I),I#1,NP)                         FFE  120
             READ INPUT TAPE 3,00202,NV                                      FFE  121
             WRITE OUTPUT TAPE 9,00502,NV                                    FFE  122
             NM#(NV*(NV+1))/2                                                FFE  123
             READ INPUT TAPE 3,02002,(PM(K),K#1,NM)                          FFE  124
02002        FORMAT (8E15.8)                                                 FFE  125
                                                                             FFE  126
C      PUT OUT INPUT PARAMETERS                                              FFE  127
02101 WRITE OUTPUT TAPE 9,02102                                              FFE  128
02102 FORMAT (11H0INPUT DATA/21H0  I      P(I)  KII(I)/1H )                  FFE  129
      DO 02104 I#1,NP                                                        FFE  130
                                                                             FFE  131
02104     WRITE OUTPUT TAPE 9,02105,I,P(I),KII(I)                            FFE  132
02105     FORMAT (1H I3,F10.4,I4)                                            FFE  133
                                                                             FFE  134
C      READ AND PUT OUT CELL PARAMETERS                                      FFE  135
      READ INPUT TAPE 10,02202,(A(I),I#1,6)                                  FFE  136
```

```
02202 FORMAT (6F9.4)                                                    FFE  137
      WRITE OUTPUT TAPE 9,00104,(TITLE(I),I#1,12)                       FFE  138
      WRITE OUTPUT TAPE 9,02205,(A(I),I#1,6)                            FFE  139
02205 FORMAT(16H0CELL PARAMETERS/1H06F11.4)                             FFE  140
      IF(IAM-1)03401,02401,02701                                        FFE  141
                                                                        FFE  142
C        READ STANDARD ERRORS OF CELL PARAMETERS                        FFE  143
02401    DO 02402 I#1,21                                                FFE  144
                                                                        FFE  145
02402       AM(I)#0.0                                                   FFE  146
                                                                        FFE  147
         READ INPUT TAPE 10,02202,AM(1),AM(7),AM(12),AM(16),            FFE  148
     1                                   AM(19),AM(21)                  FFE  149
         WRITE OUTPUT TAPE 9,02503,AM(1),AM(7),AM(12),AM(16),           FFE  150
     1                                   AM(19),AM(21)                  FFE  151
02503    FORMAT (49H0STANDARD ERRORS, RESPECTIVELY, OF THE ABOVE CELL   FFE  152
     1      11H PARAMETERS/1H06F11.4)                                   FFE  153
         DO 02602 I#1,21                                                FFE  154
                                                                        FFE  155
02602       AM(I)#AM(I)*AM(I)                                           FFE  156
                                                                        FFE  157
         GO TO 03201                                                    FFE  158
                                                                        FFE  159
C        READ VARIANCE-COVARIANCE MATRIX FOR CELL PARAMETERS            FFE  160
02701    READ INPUT TAPE 10,00603,(AM(I),I#1,21)                        FFE  161
         WRITE OUTPUT TAPE 9,2703                                       FFE  162
02703    FORMAT (47H0VARIANCE-COVARIANCE MATRIX FOR CELL PARAMETERS)    FFE  163
         IJ#1                                                           FFE  164
         DO 03101 I#1,6                                                 FFE  165
                                                                        FFE  166
            DO 02902 J#1,6                                              FFE  167
                                                                        FFE  168
02902          ROW(J)#0.0                                               FFE  169
                                                                        FFE  170
            DO 03003 J#1,6                                              FFE  171
                                                                        FFE  172
               ROW(J)#AM(IJ)                                            FFE  173
03003          IJ#IJ+1                                                  FFE  174
                                                                        FFE  175
03101       WRITE OUTPUT TAPE 9,03102,(ROW(J),J#1,6)                    FFE  176
03102       FORMAT (1H06F11.4)                                          FFE  177
                                                                        FFE  178
C        COMPUTE CELL PARAMETER INCREMENTS USED TO OBTAIN DERIVATIVES   FFE  179
03201    K#1                                                            FFE  180
         L#6                                                            FFE  181
         DO 03303 I#1,6                                                 FFE  182
                                                                        FFE  183
            DA(I)#(0.01)*SQRTF(AM(K))                                   FFE  184
            K#K+L                                                       FFE  185
03303       L#L-1                                                       FFE  186
                                                                        FFE  187
03401 IF(NS)03701,03701,03601                                           FFE  188
                                                                        FFE  189
C        READ AND PUT OUT SYMMETRY TRANSFORMATIONS                      FFE  190
03601    READ INPUT TAPE 10,03602,((TS(I,J),(IS(K,I,J),K#1,2),I#1,3),   FFE  191
     1                                                  J#1,NS)         FFE  192
03602    FORMAT (F11.6,2I2,F11.6,2I2,F11.6,2I2)                         FFE  193
         WRITE OUTPUT TAPE 9,03604                                      FFE  194
03604    FORMAT (21H0SYMMETRY INFORMATION/19H0      TRANSFORMED X       FFE  195
     1      48H            TRANSFORMED Y            TRANSFORMED Z/1H )  FFE  196
         WRITE OUTPUT TAPE 9,03608,((TS(I,J),(IS(K,I,J),K#1,2),I#1,3),  FFE  197
     1                                                  J#1,NS)         FFE  198
03608    FORMAT (1H F13.6,2I2,F20.6,2I2,F20.6,2I2)                      FFE  199
                                                                        FFE  200
03701 IF(IPM)03801,04001,03801                                          FFE  201
                                                                        FFE  202
C        COMPUTE PARAMETER INCREMENTS USED TO OBTAIN DERIVATIVES        FFE  203
03801    K#1                                                            FFE  204
         L#NV                                                           FFE  205
         DO 03903 I#1,NV                                                FFE  206
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                                                                        FFE  207
            DP(I)#(0.01)*SQRTF(PM(K))                                   FFE  208
            K#K+L                                                       FFE  209
03903       L#L-1                                                       FFE  210
                                                                        FFE  211
04001 WRITE OUTPUT TAPE 9,04002,(TITLE(I),I#1,12)                       FFE  212
04002 FORMAT (1H112A6/1H )                                              FFE  213
                                                                        FFE  214
C        READ ONE SET OF INSTRUCTIONS                                   FFE  215
04101    K#1                                                            FFE  216
         DO 04501 I#1,10                                                FFE  217
                                                                        FFE  218
            L#K+23                                                      FFE  219
            READ INPUT TAPE 10,00202,(IN(J),J#K,L)                      FFE  220
            IF(IN(L))04501,04601,04501                                  FFE  221
                                                                        FFE  222
04501       K#L                                                         FFE  223
                                                                        FFE  224
04601    IF(IN(1))04801,04701,04801                                     FFE  225
                                                                        FFE  226
C           END OF JOB                                                  FFE  227
04701       CALL EXIT                                                   FFE  228
                                                                        FFE  229
04801    IF(IN(1)-INSAVE)04901,05001,04901                              FFE  230
                                                                        FFE  231
C           PUT OUT HEADING FOR NEW TYPE OF FUNCTION                    FFE  232
04901       CALL HED1(IN(1))                                            FFE  233
                                                                        FFE  234
05001    INSAVE#IN(1)                                                   FFE  235
         IF(IN(1)-100)05101,05101,05201                                 FFE  236
                                                                        FFE  237
C           COMPUTE SINGLE-VALUED FUNCTION                              FFE  238
05101       CALL SUB19                                                  FFE  239
            GO TO 04101                                                 FFE  240
                                                                        FFE  241
C           COMPUTE MULTIPLE-VALUED FUNCTION                            FFE  242
05201       CALL SUB21                                                  FFE  243
            GO TO 04101                                                 FFE  244
                                                                        FFE  245
      END(0,1,0,0,0)                                                    FFE  246
*TYPE(FORTRAN)                                                          FFE  247
C     COMPUTE ALL DISTANCES BETWEEN TWO ASYMMETRIC UNITS                FFE  248
      SUBROUTINE SUB8                                                   FFE  249
                                                                        FFE  250
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NO,INSAVE   FFE  251
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  252
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  253
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  254
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  255
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  256
                                                                        FFE  257
C     SET MAXIMUM DISTANCE ACCEPTED                                     FFE  258
      IF(IN(6))107,107,111                                              FFE  259
                                                                        FFE  260
  107    DMAX#4.0                                                       FFE  261
         GOTO113                                                        FFE  262
                                                                        FFE  263
  111    DMAX#FLOATF(IN(6))/10.0                                        FFE  264
                                                                        FFE  265
  113 NA#IN(2)                                                          FFE  266
      IF(NA)217,217,117                                                 FFE  267
                                                                        FFE  268
C     START LOOP FOR FIRST ATOM                                         FFE  269
  117 DO215I#1,NA                                                       FFE  270
                                                                        FFE  271
         IN(2)#I                                                        FFE  272
                                                                        FFE  273
C        START LOOP FOR SECOND ATOM                                     FFE  274
         DO213J#1,NA                                                    FFE  275
                                                                        FFE  276
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C           TEST TO AVOID DUPLICATION                                   FFE  277
            IF(IN(3)-IN(5))201,135,201                                  FFE  278
                                                                        FFE  279
  135          IF(J-I)201,215,215                                       FFE  280
                                                                        FFE  281
  201       IN(4)#J                                                     FFE  282
            NG#0                                                        FFE  283
                                                                        FFE  284
C           COMPUTE AND TEST DISTANCE                                   FFE  285
            CALL FUNI(IN(1))                                            FFE  286
            IF(FX-DMAX)209,209,213                                      FFE  287
                                                                        FFE  288
C              COMPUTE ERROR AND PUT OUT RESULTS                        FFE  289
  209          F#FX                                                     FFE  290
               CALLSUB13                                                FFE  291
                                                                        FFE  292
  213       CONTINUE                                                    FFE  293
C           END LOOP FOR SECOND ATOM                                    FFE  294
                                                                        FFE  295
  215    CONTINUE                                                       FFE  296
C        END LOOP FOR FIRST ATOM                                        FFE  297
                                                                        FFE  298
  217 RETURN                                                            FFE  299
      END(0,1,0,0,0)                                                    FFE  300
*TYPE(FORTRAN)                                                          FFE  301
C     MULTIVALUED FUNCTIONS 7, 8, AND 9                                 FFE  302
      SUBROUTINE SUB10                                                  FFE  303
                                                                        FFE  304
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  305
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE  306
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  307
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  308
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  309
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  310
                                                                        FFE  311
C     START LOOP THRU PRINCIPAL AXES                                    FFE  312
      DO109I#1,3                                                        FFE  313
                                                                        FFE  314
         IN(4)#I                                                        FFE  315
                                                                        FFE  316
C        COMPUTE AND PUT OUT FUNCTION AND ERROR                         FFE  317
  109    CALLSUB19                                                      FFE  318
                                                                        FFE  319
      RETURN                                                            FFE  320
      END(0,1,0,0,0)                                                    FFE  321
*TYPE(FORTRAN)                                                          FFE  322
C     MULTIVALUED FUNCTIONS 10 AND 11                                   FFE  323
      SUBROUTINE SUB11                                                  FFE  324
                                                                        FFE  325
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  326
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE  327
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  328
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  329
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  330
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  331
                                                                        FFE  332
C     START LOOP THRU PRINCIPAL AXES                                    FFE  333
      DO113I#1,3                                                        FFE  334
                                                                        FFE  335
         IN(4)#I                                                        FFE  336
                                                                        FFE  337
C        START LOOP THRU REFERENCE AXES                                 FFE  338
         DO113J#1,3                                                     FFE  339
                                                                        FFE  340
            IN(5)#J                                                     FFE  341
                                                                        FFE  342
C           COMPUTE AND PUT OUT FUNCTION AND ERROR                      FFE  343
  113       CALLSUB19                                                   FFE  344
                                                                        FFE  345
      RETURN                                                            FFE  346
```

```
      END(0,1,0,0,0)                                                    FFE  347
*TYPE(FORTRAN)                                                          FFE  348
C     ERROR CALCULATION AND OUTPUT                                      FFE  349
      SUBROUTINE SUB13                                                  FFE  350
                                                                        FFE  351
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  352
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  353
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  354
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  355
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  356
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  357
                                                                        FFE  358
C     PUT OUT FUNCTION DESCRIPTION                                      FFE  359
      CALL OUTI(IN(1))                                                  FFE  360
      IF(NG)107,113,107                                                 FFE  361
                                                                        FFE  362
C        PUT OUT ERROR INDICATOR IF NOT ZERO                            FFE  363
  107    WRITE OUTPUT TAPE 9,109,NG                                     FFE  364
  109    FORMAT (1H 51X,3H***I3)                                        FFE  365
         GO TO 723                                                      FFE  366
                                                                        FFE  367
  113 VARA#0.0                                                          FFE  368
      VARP#0.0                                                          FFE  369
      IF(IAM)119,313,119                                                FFE  370
                                                                        FFE  371
C        COMPUTE DERIVATIVES WITH RESPECT TO CELL PARAMETERS            FFE  372
  119    DO 211 I#1,6                                                   FFE  373
                                                                        FFE  374
            IF(DA(I))201,123,201                                        FFE  375
                                                                        FFE  376
  123          DFDA(I)#0.0                                              FFE  377
               GO TO 211                                                FFE  378
                                                                        FFE  379
  201          SAVEA#A(I)                                               FFE  380
               A(I)#A(I)+DA(I)                                          FFE  381
               CALL FUNI(IN(1))                                         FFE  382
               A(I)#SAVEA                                               FFE  383
               DFDA(I)#(FX-F)/DA(I)                                     FFE  384
                                                                        FFE  385
  211       CONTINUE                                                    FFE  386
                                                                        FFE  387
C        COMPUTE VARIANCE BASED ON CELL PARAMETERS                      FFE  388
         K#1                                                            FFE  389
         L#6                                                            FFE  390
         DO 311 I#1,6                                                   FFE  391
                                                                        FFE  392
            IF(DFDA(I))225,221,225                                      FFE  393
                                                                        FFE  394
  221          K#K+L                                                    FFE  395
               GO TO 311                                                FFE  396
                                                                        FFE  397
  225          C#1.0                                                    FFE  398
               DO 309 J#1,6                                             FFE  399
                                                                        FFE  400
                  IF(DFDA(J))305,307,305                                FFE  401
                                                                        FFE  402
  305                VARA#VARA+C*DFDA(I)*DFDA(J)*AM(K)                  FFE  403
                                                                        FFE  404
  307             K#K+1                                                 FFE  405
  309             C#2.0                                                 FFE  406
                                                                        FFE  407
  311       L#L-1                                                       FFE  408
                                                                        FFE  409
  313 IF(IPM)315,615,315                                                FFE  410
                                                                        FFE  411
C        SELECT DERIVATIVES TO BE COMPUTED                              FFE  412
  315    DO 319 I#1,NP                                                  FFE  413
                                                                        FFE  414
  319       KI2(I)#0                                                    FFE  415
                                                                        FFE  416
```

```
      CALL PRFI(IN(I))
C     COMPUTE DERIVATIVES WITH RESPECT TO STRUCTURE PARAMETERS
      J#0
      DO 513 I#1,NV
  403    J#J+1
         IF(KI1(J))407,403,407
  407    IF(KI2(J))413,409,413
  409       DFDP(I)#0.0
            GO TO 513
  413       IF(DP(I))501,409,501
  501       SAVEP#P(J)
            P(J)#P(J)+DP(I)
            CALL FUNI(IN(I))
            P(J)#SAVEP
            DFDP(I)#(FX-F)/DP(I)
            LNZ#I
  513    CONTINUE
C     COMPUTE VARIANCE BASED ON STRUCTURE PARAMETERS
      KK#1
      KKD#NV
      DO 613 I#1,LNZ
         IF(DFDP(I))523,612,523
  523       K#KK
            C#1.0
            DO 611 J#1,LNZ
               IF(DFDP(J))607,609,607
  607             VARP#VARP+C*DFDP(I)*DFDP(J)*PM(K)
  609          K#K+1
  611          C#2.0
  612    KK#KK+KKD
  613    KKD#KKD-1
  615 IF(NG)617,623,617
C     PUT OUT ERROR INDICATOR IF NOT ZERO
  617 WRITE OUTPUT TAPE 9,619,F,NG
  619 FORMAT (1H 48X,F9.4,6X,3H***I3)
      GO TO 723
C   COMPUTE STANDARD ERRORS AND PUT OUT RESULTS
  623 EI#SQRTF(VARP)
      E#SQRTF(VARP+VARA)
      IF(IPM)703,705,703
  703 IF(IAM)707,713,707
  705 IF(IAM)713,719,713
  707    WRITE OUTPUT TAPE 9,709,F,E,EI
  709    FORMAT (1H 48X,F9.4,5H +OR-F7.4,2H (F7.4,1H))
         GO TO 723
  713    WRITE OUTPUT TAPE 9,715,F,E
  715    FORMAT (1H 48X,F9.4,5H +OR-F7.4)
         GO TO 723
```

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  719        WRITE OUTPUT TAPE 9,721,F                                    FFE  487
  721        FORMAT (1H 48X,F9.4)                                         FFE  488
                                                                          FFE  489
  723 RETURN                                                              FFE  490
      END(0,1,0,0,0)                                                      FFE  491
*TYPE(FORTRAN)                                                            FFE  492
C     FUNCTION AND ERROR CALCULATION                                      FFE  493
      SUBROUTINE SUB19                                                    FFE  494
                                                                          FFE  495
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE     FFE  496
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP    FFE  497
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2   FFE  498
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)        FFE  499
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  500
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                           FFE  501
                                                                          FFE  502
      NG#0                                                                FFE  503
      CALL FUNI(IN(1))                                                    FFE  504
      F#FX                                                                FFE  505
      CALLSUB13                                                           FFE  506
      RETURN                                                              FFE  507
      END(0,1,0,0,0)                                                      FFE  508
*TYPE(FORTRAN)                                                            FFE  509
C     COMPUTE MULTIVALUED FUNCTIONS                                       FFE  510
*     SUBROUTINE SUB21                                                    FFE  511
                                                                          FFE  512
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE     FFE  513
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP    FFE  514
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2   FFE  515
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)        FFE  516
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  517
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                           FFE  518
                                                                          FFE  519
C     UNPACK INSTRUCTION NUMBER                                           FFE  520
      IH#IN(1)/100                                                        FFE  521
      IN(1)#IN(1)-100*IH                                                  FFE  522
                                                                          FFE  523
C     TRANSFER TO APPROPRIATE SECTION                                     FFE  524
      IF(IN(1)-11)111,111,319                                             FFE  525
  111 IF(IN(1)-9)113,113,305                                              FFE  526
  113 IF(IN(1)-6)115,115,215                                              FFE  527
  115 IF(IN(1)-1)117,117,319                                              FFE  528
                                                                          FFE  529
  117    IF(IH-1)119,119,123                                              FFE  530
                                                                          FFE  531
C           COMPUTE ALL DISTANCES BETWEEN TWO UNITS                       FFE  532
  119       CALLSUB8                                                      FFE  533
            GOTO319                                                       FFE  534
                                                                          FFE  535
C           COMPUTE DISTANCES INVOLVING BASIC UNIT AND ALL OTHERS         FFE  536
  123       NA#IN(2)                                                      FFE  537
            NSP#NS+1                                                      FFE  538
            IN(3)#0                                                       FFE  539
            DO211I#1,8                                                    FFE  540
                                                                          FFE  541
               DO211J#1,NSP                                               FFE  542
                                                                          FFE  543
                  IN(2)#NA                                                FFE  544
                  IN(5)#100*(I-1)+J-1                                     FFE  545
  211             CALLSUB8                                                FFE  546
                                                                          FFE  547
            GOTO319                                                       FFE  548
                                                                          FFE  549
  215    IF(IH-1)217,217,221                                              FFE  550
                                                                          FFE  551
C           COMPUTE FUNCTIONS INVOLVING THREE PRINCIPAL AXES              FFE  552
  217       CALLSUB10                                                     FFE  553
            GOTO319                                                       FFE  554
                                                                          FFE  555
C           COMPUTE FUNCTIONS INVOLVING THREE PRINCIPAL AXES              FFE  556
```

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C                                                   FOR ALL ATOMS
  221       NA#IN(2)
            DO301I#1,NA

               IN(2)#I
  301          CALLSUB10

            GOTO319

  305     IF(IH-1)307,307,311

C           COMPUTE FOR ALL PRINCIPAL AXES AND ALL REFERENCE AXES
  307       CALLSUB11
            GOTO319

C           COMPUTE FOR ALL PRINCIPAL AXES, ALL REFERENCE AXES,
C                                                AND ALL ATOMS
  311       NA#IN(2)
            DO317I#1,NA

               IN(2)#I
  317          CALLSUB11

  319 RETURN
      END(0,1,0,0,0)
*TYPE(FORTRAN)
C     SELECT THE HED SUBROUTINE TO BE ENTERED
      SUBROUTINE HED1(I)
      K#XMODF(I,100)
      IF(K)160,160,4

    4 IF(K-15)8,8,160

    8 GO TO (10,20,30,40,50,60,70,80,90,100,110,120,130,140,150),K

   10     CALL HED1
          GO TO 160

   20     CALL HED2
          GO TO 160

   30     CALL HED3
          GO TO 160

   40     CALL HED4
          GO TO 160

   50     CALL HED5
          GO TO 160

   60     CALL HED6
          GO TO 160

   70     CALL HED7
          GO TO 160

   80     CALL HED8
          GO TO 160

   90     CALL HED9
          GO TO 160

  100     CALL HED10
          GO TO 160

  110     CALL HED11
          GO TO 160

  120     CALL HED12
          GO TO 160
```

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                                                                        FFE  627
  130     CALL HED13                                                    FFE  628
          GO TO 160                                                     FFE  629
                                                                        FFE  630
  140     CALL HED14                                                    FFE  631
          GO TO 160                                                     FFE  632
                                                                        FFE  633
  150     CALL HED15                                                    FFE  634
                                                                        FFE  635
  160 RETURN                                                            FFE  636
      END(0,1,0,0,0)                                                    FFE  637
*TYPE (FORTRAN)                                                         FFE  638
C     SELECT THE PRE SUBROUTINE TO BE ENTERED                           FFE  639
      SUBROUTINE PREI(I)                                                FFE  640
    4 IF(I)160,160,6                                                    FFE  641
                                                                        FFE  642
    6 IF(I-15)8,8,160                                                   FFE  643
                                                                        FFE  644
    8 GO TO (10,20,30,40,30,60,70,80,80,100,100,120,70,140,140),I       FFE  645
                                                                        FFE  646
   10     CALL PRE1                                                    FFE  647
          GO TO 160                                                     FFE  648
                                                                        FFE  649
   20     CALL PRE2                                                    FFE  650
          GO TO 160                                                     FFE  651
                                                                        FFE  652
   30     CALL PRE3                                                    FFE  653
          GO TO 160                                                     FFE  654
                                                                        FFE  655
   40     CALL PRE4                                                    FFE  656
          GO TO 160                                                     FFE  657
                                                                        FFE  658
   60     CALL PRE6                                                    FFE  659
          GO TO 160                                                     FFE  660
                                                                        FFE  661
   70     CALL PRE7                                                    FFE  662
          GO TO 160                                                     FFE  663
                                                                        FFE  664
   80     CALL PRE8                                                    FFE  665
          GO TO 160                                                     FFE  666
                                                                        FFE  667
                                                                        FFE  668
  100     CALL PRE10                                                    FFE  669
          GO TO 160                                                     FFE  670
                                                                        FFE  671
  120     CALL PRE12                                                    FFE  672
          GO TO 160                                                     FFE  673
                                                                        FFE  674
  140     CALL PRE14                                                    FFE  675
                                                                        FFE  676
  160 RETURN                                                            FFE  677
      END(0,1,0,0,0)                                                    FFE  678
*TYPE (FORTRAN)                                                         FFE  679
C     SELECT THE FUN SUBROUTINE TO BE ENTERED                           FFE  680
      SUBROUTINE FUNI(I)                                                FFE  681
                                                                        FFE  682
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  683
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVFA,SAVFP,VARA,VARP,FI,F,IH,NSP  FFE  684
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  685
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  686
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  687
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  688
                                                                        FFE  689
      CALL SETA(A)                                                      FFE  690
      CALL SETP(P)                                                      FFE  691
      IF(I)6,6,5                                                        FFE  692
                                                                        FFE  693
    5 IF(I-15)8,8,6                                                     FFE  694
                                                                        FFE  695
    6     NG#11                                                         FFE  696
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      GO TO 160                                                         FFE  697
                                                                        FFE  698
    8 GO TO (10,20,30,40,50,60,70,80,90,100,110,120,130,140,150),I      FFE  699
                                                                        FFE  700
   10 CALL FUN1                                                         FFE  701
      GO TO 160                                                         FFE  702
                                                                        FFE  703
   20 CALL FUN2                                                         FFE  704
      GO TO 160                                                         FFE  705
                                                                        FFE  706
   30 CALL FUN3                                                         FFE  707
      GO TO 160                                                         FFE  708
                                                                        FFE  709
   40 CALL FUN4                                                         FFE  710
      GO TO 160                                                         FFE  711
                                                                        FFE  712
   50 CALL FUN5                                                         FFE  713
      GO TO 160                                                         FFE  714
                                                                        FFE  715
   60 CALL FUN6                                                         FFE  716
      GO TO 160                                                         FFE  717
                                                                        FFE  718
   70 CALL FUN7                                                         FFE  719
      GO TO 160                                                         FFE  720
                                                                        FFE  721
   80 CALL FUN8                                                         FFE  722
      GO TO 160                                                         FFE  723
                                                                        FFE  724
   90 CALL FUN9                                                         FFE  725
      GO TO 160                                                         FFE  726
                                                                        FFE  727
  100 CALL FUN10                                                        FFE  728
      GO TO 160                                                         FFE  729
                                                                        FFE  730
  110 CALL FUN11                                                        FFE  731
      GO TO 160                                                         FFE  732
                                                                        FFE  733
  120 CALL FUN12                                                        FFE  734
      GO TO 160                                                         FFE  735
                                                                        FFE  736
  130 CALL FUN13                                                        FFE  737
      GO TO 160                                                         FFE  738
                                                                        FFE  739
  140 CALL FUN14                                                        FFE  740
      GO TO 160                                                         FFE  741
                                                                        FFE  742
  150 CALL FUN15                                                        FFE  743
                                                                        FFE  744
  160 RETURN                                                            FFE  745
      END(0,1,0,0,0)                                                    FFE  746
*TYPE (FORTRAN)                                                         FFE  747
C     SELECT THE OUT SUBROUTINE TO BE ENTERED                           FFE  748
      SUBROUTINE OUTI(I)                                                FFE  749
    4 IF(I)160,160,6                                                    FFE  750
                                                                        FFE  751
    6 IF(I-15)8,8,160                                                   FFE  752
                                                                        FFE  753
    8 GO TO (10,20,30,40,30,60,70,80,80,100,100,120,130,10,10),I        FFE  754
                                                                        FFE  755
   10 CALL OUT1                                                         FFE  756
      GO TO 160                                                         FFE  757
                                                                        FFE  758
   20 CALL OUT2                                                         FFE  759
      GO TO 160                                                         FFE  760
                                                                        FFE  761
   30 CALL OUT3                                                         FFE  762
      GO TO 160                                                         FFE  763
                                                                        FFE  764
   40 CALL OUT4                                                         FFE  765
      GO TO 160                                                         FFE  766
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                                                                        FFE  767
   60     CALL OUT6                                                     FFE  768
          GO TO 160                                                     FFE  769
                                                                        FFE  770
   70     CALL OUT7                                                     FFE  771
          GO TO 160                                                     FFE  772
                                                                        FFE  773
   80     CALL OUT8                                                     FFE  774
          GO TO 160                                                     FFE  775
                                                                        FFE  776
  100     CALL OUT10                                                    FFE  777
          GO TO 160                                                     FFE  778
                                                                        FFE  779
  120     CALL OUT12                                                    FFE  780
          GO TO 160                                                     FFE  781
                                                                        FFE  782
  130     CALL OUT13                                                    FFE  783
                                                                        FFE  784
  160 RETURN                                                            FFE  785
      END(0,1,0,0,0)                                                    FFE  786
*TYPE(FORTRAN)                                                          FFE  787
C     SET KEY WORDS FOR ATOM COORDINATES                                FFE  788
      SUBROUTINE SETKX(I)                                               FFE  789
C     I#IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER       FFE  790
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  791
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE  792
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  793
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  794
      DIMENSION DFDA(6),IN(2311),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  795
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  796
      IF(I)119,119,111                                                  FFE  797
  111 J#JX+JXP*(I-1)                                                    FFE  798
      KI2(J)#1                                                          FFE  799
      KI2(J+1)#1                                                        FFE  800
      KI2(J+2)#1                                                        FFE  801
  119 RETURN                                                            FFE  802
      END(0,1,0,0,0)                                                    FFE  803
*TYPE(FORTRAN)                                                          FFE  804
C     SET KEY WORDS FOR ATOM BETAS                                      FFE  805
      SUBROUTINE SETKB(I)                                               FFE  806
C     I#IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER       FFE  807
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  808
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE  809
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  810
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  811
      DIMENSION DFDA(6),IN(2311),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  812
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  813
      IF(I)119,119,111                                                  FFE  814
  111 J#JB+JBP*(I-1)                                                    FFE  815
      DO 117 K#1,6                                                      FFE  816
      KI2(J)#1                                                          FFE  817
  117 J#J+1                                                             FFE  818
  119 RETURN                                                            FFE  819
      END(0,1,0,0,0)                                                    FFE  820
*TYPE(FORTRAN)                                                          FFE  821
C     STORE METRIC TENSOR                                               FFE  822
      SUBROUTINE STOAA                                                  FFE  823
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  824
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE  825
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  826
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  827
      DIMENSION DFDA(6),IN(2311),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  828
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  829
      AA(1,1)#A(1)*A(1)                                                 FFE  830
      AA(2,2)#A(2)*A(2)                                                 FFE  831
      AA(3,3)#A(3)*A(3)                                                 FFE  832
      AA(1,2)#A(1)*A(2)*A(6)                                            FFE  833
      AA(2,1)#AA(1,2)                                                   FFE  834
      AA(1,3)#A(1)*A(3)*A(5)                                            FFE  835
      AA(3,1)#AA(1,3)                                                   FFE  836
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      AA(2,3)#A(2)*A(3)*A(4)                                            FFE  837
      AA(3,2)#AA(2,3)                                                   FFE  838
      RETURN                                                            FFE  839
      END(0,1,0,0,0)                                                    FFE  840
*TYPE(FORTRAN)                                                          FFE  841
C     STORE RECIPROCAL METRIC TENSOR                                    FFE  842
      SUBROUTINE STOBB                                                  FFE  843
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  844
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  845
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  846
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  847
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  848
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  849
      DIMENSIONAI(6),CI(6),BBII(3),BBJK(3)                              FFE  850
      DO12I#1,3                                                         FFE  851
      IF(A(I))111,111,115                                               FFE  852
  111 NG#6                                                              FFE  853
      GOTO225                                                           FFE  854
  115 AI(I)#A(I)                                                        FFE  855
      AI(I+3)#A(I)                                                      FFE  856
      CI(I)#A(I+3)                                                      FFE  857
  121 CI(I+3)#A(I+3)                                                    FFE  858
      X#1.0/(AI(1)*AI(2)*AI(3)*(1.0-CI(1)*CI(1)-CI(2)*CI(2)             FFE  859
     1-CI(3)*CI(3)+2.0*CI(1)*CI(2)*CI(3)))                              FFE  860
      DO205I#1,3                                                        FFE  861
      BBII(I)#X*(1.0-CI(I)*CI(I))*AI(I+1)*AI(I+2)/AI(I)                 FFE  862
  205 BBJK(I)#X*AI(I)*(CI(I+1)*CI(I+2)-CI(I))                           FFE  863
      BB(1,1)#BBII(1)                                                   FFE  864
      BB(1,2)#BBJK(3)                                                   FFE  865
      BB(1,3)#BBJK(2)                                                   FFE  866
      BB(2,1)#BBJK(3)                                                   FFE  867
      BB(2,2)#BBII(2)                                                   FFE  868
      BB(2,3)#BBJK(1)                                                   FFE  869
      BB(3,1)#BBJK(2)                                                   FFE  870
      BB(3,2)#BBJK(1)                                                   FFE  871
      BB(3,3)#BBII(3)                                                   FFE  872
  225 RETURN                                                            FFE  873
      END(0,1,0,0,0)                                                    FFE  874
*TYPE(FORTRAN)                                                          FFE  875
C     ATOM COORDINATE SUBROUTINE                                        FFE  876
      SUBROUTINE ATOM(I,Z)                                              FFE  877
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  878
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  879
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  880
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  881
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  882
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  883
      DIMENSIONI(2),X(3),Y(3),Z(3)                                      FFE  884
      IF(I(1))109,109,117                                               FFE  885
  109 X(1)#0.0                                                          FFE  886
      X(2)#0.0                                                          FFE  887
      X(3)#0.0                                                          FFE  888
      GOTO125                                                           FFE  889
  117 K#JXP*(I(1)-1)+JX                                                 FFE  890
      IF(K+2-NP)119,119,503                                             FFE  891
  503 NG#5                                                              FFE  892
      GOTO325                                                           FFE  893
  119 DO123J#1,3                                                        FFE  894
      X(J)#P(K)                                                         FFE  895
  123 K#K+1                                                             FFE  896
  125 KC#I(2)/100                                                       FFE  897
      KS#I(2)-100*KC                                                    FFE  898
      IF(KS-NS)203,203,403                                              FFE  899
  403 NG#1                                                              FFE  900
      GOTO325                                                           FFE  901
  203 IF(KS)403,205,213                                                 FFE  902
  205 Y(1)#X(1)                                                         FFE  903
      Y(2)#X(2)                                                         FFE  904
      Y(3)#X(3)                                                         FFE  905
      GOTO311                                                           FFE  906
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  213 DO215J#1,3                                                        FFE  907
  215 Y(J)#TS(J,KS)                                                     FFE  908
      DO309K#1,3                                                        FFE  909
      DO307J#1,2                                                        FFE  910
      L#IS(J,K,KS)                                                      FFE  911
      IF(L)225,307,305                                                  FFE  912
  225 L#-L                                                              FFE  913
      Y(K)#Y(K)-X(L)                                                    FFE  914
      GOTO307                                                           FFE  915
  305 Y(K)#Y(K)+X(L)                                                    FFE  916
  307 CONTINUE                                                          FFE  917
  309 CONTINUE                                                          FFE  918
  311 KC4#KC/4                                                          FFE  919
      KC3#KC-4*KC4                                                      FFE  920
      KC2#KC3/2                                                         FFE  921
      KC1#KC3-2*KC2                                                     FFE  922
      Z(1)#Y(1)-FLOATF(KC1)                                             FFE  923
      Z(2)#Y(2)-FLOATF(KC2)                                             FFE  924
      Z(3)#Y(3)-FLOATF(KC4)                                             FFE  925
  325 RETURN                                                            FFE  926
      END(0,1,0,0,0)                                                    FFE  927
*TYPE(FORTRAN)                                                          FFE  928
C     STORE TRANSFORMED ANISOTROPIC TEMP FACTOR MATRIX                  FFE  929
C     INS IS ATOM DESCRIPTION, Z IS TRANSFORMED MATRIX                  FFE  930
      SUBROUTINE BETA(INS,Z)                                            FFE  931
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  932
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  933
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  934
      DIMENSION TITLE(12),PM(201,00),DP(200),DFDP(200),AM(21),DA(6)     FFE  935
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  936
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  937
      DIMENSIONINS(2),Z(3,3),B1(6),B2(9)                                FFE  938
      IF(ITF-1)100,111,115                                              FFE  939
  100 IF(JBP-6)111,115,115                                              FFE  940
  111 NG#4                                                              FFE  941
      GOTO423                                                           FFE  942
  115 KS#XMODF(INS(2),100)                                              FFE  943
      IF(KS)121,119,119                                                 FFE  944
  119 IF(KS-NS)125,125,121                                              FFE  945
  121 NG#1                                                              FFE  946
      GOTO423                                                           FFE  947
  125 IF(INS(1))211,201,207                                             FFE  948
  201 DO203I#1,6                                                        FFE  949
  203 B1(I)#0.0                                                         FFE  950
      GOTO221                                                           FFE  951
  207 J#JB+JBP*(INS(1)-1)                                               FFE  952
      IF(J+5-NP)215,215,211                                             FFE  953
  211 NG#5                                                              FFE  954
      GOTO423                                                           FFE  955
  215 DO219I#1,6                                                        FFE  956
      B1(I)#P(J)                                                        FFE  957
  219 J#J+1                                                             FFE  958
  221 B2(1)#B1(1)                                                       FFE  959
      B2(2)#B1(4)                                                       FFE  960
      B2(3)#B1(5)                                                       FFE  961
      B2(4)#B1(2)                                                       FFE  962
      B2(6)#B1(6)                                                       FFE  963
      B2(9)#B1(3)                                                       FFE  964
      DO421I#1,3                                                        FFE  965
      DO419J#1,3                                                        FFE  966
      IF(KS)121,313,319                                                 FFE  967
  313 M#I*J                                                             FFE  968
      B3#B2(M)                                                          FFE  969
      GOTO415                                                           FFE  970
  319 B3#0.0                                                            FFE  971
      DO413K#1,2                                                        FFE  972
      DO411L#1,2                                                        FFE  973
      M#IS(K,I,KS)*IS(L,J,KS)                                           FFE  974
      IF(M)407,411,403                                                  FFE  975
  403 B3#B3+B2(M)                                                       FFE  976
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      GOTO411                                                           FFE  977
  407 M#-M                                                              FFE  978
      B3#B3-B2(M)                                                       FFE  979
  411 CONTINUE                                                          FFE  980
  413 CONTINUE                                                          FFE  981
  415 Z(I,J)#B3                                                         FFE  982
      Z(J,I)#B3                                                         FFE  983
  419 CONTINUE                                                          FFE  984
  421 CONTINUE                                                          FFE  985
  423 RETURN                                                            FFE  986
      END(0,1,0,0,0)                                                    FFE  987
*TYPE(FORTRAN)                                                          FFE  988
C     MULTIPLY TWO MATRICES                                             FFE  989
C     Z(3,3)#X(3,3)*Y(3,3)                                              FFE  990
      SUBROUTINE MM(X,Y,Z)                                              FFE  991
      DIMENSIONX(3,3),Y(3,3),Z(3,3)                                     FFE  992
      DO117I#1,3                                                        FFE  993
      DO117K#1,3                                                        FFE  994
      Z(I,K)#0.0                                                        FFE  995
      DO117J#1,3                                                        FFE  996
  117 Z(I,K)#Z(I,K)+X(I,J)*Y(J,K)                                       FFE  997
      RETURN                                                            FFE  998
      END(0,1,0,0,0)                                                    FFE  999
*TYPE(FORTRAN)                                                          FFE 1000
C     MATRIX * VECTOR                                                   FFE 1001
C     Z(3)#X(3,3)*Y(3)                                                  FFE 1002
      SUBROUTINE MV(X,Y,Z)                                              FFE 1003
      DIMENSIONX(3,3),Y(3),Z(3)                                         FFE 1004
      DO113I#1,3                                                        FFE 1005
      Z(I)#0.0                                                          FFE 1006
      DO113J#1,3                                                        FFE 1007
  113 Z(I)#Z(I)+X(I,J)*Y(J)                                             FFE 1008
      RETURN                                                            FFE 1009
      END(0,1,0,0,0)                                                    FFE 1010
*TYPE(FORTRAN)                                                          FFE 1011
C     TRANSPOSED VECTOR TIMES MATRIX                                    FFE 1012
C     Z(3)#X(3)*Y(3,3)                                                  FFE 1013
      SUBROUTINE VM(X,Y,Z)                                              FFE 1014
      )IMENSIONX(3),Y(3,3),Z(3)                                         FFE 1015
      DO115J#1,3                                                        FFE 1016
      Z(J)#0.0                                                          FFE 1017
      DO115I#1,3                                                        FFE 1018
  115 Z(J)#Z(J)+X(I)*Y(I,J)                                             FFE 1019
      RETURN                                                            FFE 1020
      END(0,1,0,0,0)                                                    FFE 1021
*TYPE(FORTRAN)                                                          FFE 1022
C     TRANSPOSED VECTOR * VECTOR                                        FFE 1023
C     VV#X(3)*Y(3)                                                      FFE 1024
      FUNCTION VV(X,Y)                                                  FFE 1025
      DIMENSIONX(3),Y(3)                                                FFE 1026
      VV#0.0                                                            FFE 1027
      DO111I#1,3                                                        FFE 1028
  111 VV#VV+X(I)*Y(I)                                                   FFE 1029
      RETURN                                                            FFE 1030
      END(0,1,0,0,0)                                                    FFE 1031
*TYPE(FORTRAN)                                                          FFE 1032
C     TRANSPOSED VECTOR * MATRIX * VECTOR                               FFE 1033
C     VMV#W(3)*X(3,3)*Y(3)                                              FFE 1034
      FUNCTION VMV(W,X,Y)                                               FFE 1035
      DIMENSIONW(3),X(3,3),Y(3),Z(3)                                    FFE 1036
      CALLMV(X,Y,Z)                                                     FFE 1037
      VMV#VV(W,Z)                                                       FFE 1038
      RETURN                                                            FFE 1039
      END(0,1,0,0,0)                                                    FFE 1040
*TYPE(FORTRAN)                                                          FFE 1041
C     VECTOR - VECTOR                                                   FFE 1042
C     Z(3)#X(3)-Y(3)                                                    FFE 1043
      SUBROUTINE DIFV(X,Y,Z)                                            FFE 1044
      DIMENSIONX(3),Y(3),Z(3)                                           FFE 1045
      DO111I#1,3                                                        FFE 1046
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  111 Z(I)#X(I)-Y(I)                                                    FFE 1047
      RETURN                                                            FFE 1048
      END(0,1,0,0,0)                                                    FFE 1049
*TYPE(FORTRAN)                                                          FFE 1050
C     COMPUTE THE SUM OF TWO VECTORS                                    FFE 1051
C     Z(3)#X(3)+Y(3)                                                    FFE 1052
      SUBROUTINE SUMV(X,Y,Z)                                            FFE 1053
      )IMENSIONX(3),Y(3),Z(3)                                           FFE 1054
      DO1111#1,3                                                        FFE 1055
  111 Z(I)#X(I)+Y(I)                                                    FFE 1056
      RETURN                                                            FFE 1057
      END(0,1,0,0,0)                                                    FFE 1058
*TYPE(FORTRAN)                                                          FFE 1059
C     COSINE OF ANGLE BETWEEN VECTORS X AND Y                           FFE 1060
      FUNCTION COSVV(X,Y)                                               FFE 1061
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1062
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1063
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1064
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1065
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1066
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1067
      DIMENSIONX(3),Y(3)                                                FFE 1068
      D#SQRTF(VMV(X,AA,X)*VMV(Y,AA,Y))                                  FFE 1069
      IF(D)111,111,115                                                  FFE 1070
  111 NG#9                                                              FFE 1071
      GOTO117                                                           FFE 1072
  115 COSVV#VMV(X,AA,Y)/D                                               FFE 1073
  117 RETURN                                                            FFE 1074
      END(0,1,0,0,0)                                                    FFE 1075
*TYPE(FORTRAN)                                                          FFE 1076
C     ARCCOS(X) IN DEGREES                                              FFE 1077
      FUNCTION ARCCOS(X)                                                FFE 1078
      ARCCOS#90.0-(57.29577951)*SIGNF(ASINF(X),X)                       FFE 1079
      RETURN                                                            FFE 1080
      END(0,1,0,0,0)                                                    FFE 1081
*TYPE(FORTRAN)                                                          FFE 1082
C     STORE A VECTOR Z NORMAL TO VECTORS X AND Y                        FFE 1083
      SUBROUTINE NORM(X,Y,Z)                                            FFE 1084
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1085
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1086
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1087
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1088
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1089
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1090
      DIMENSIONX(3),Y(3),Z(3),X1(6),Y1(6),Z1(3)                         FFE 1091
      DO115I#1,3                                                        FFE 1092
      X1(I)#X(I)                                                        FFE 1093
      X1(I+3)#X(I)                                                      FFE 1094
      Y1(I)#Y(I)                                                        FFE 1095
  115 Y1(I+3)#Y(I)                                                      FFE 1096
      DO119I#1,3                                                        FFE 1097
  119 Z1(I)#X1(I+1)*Y1(I+2)-X1(I+2)*Y1(I+1)                             FFE 1098
      CALLMV(BB,Z1,Z)                                                   FFE 1099
      RETURN                                                            FFE 1100
      END(0,1,0,0,0)                                                    FFE 1101
*TYPE(FORTRAN)                                                          FFE 1102
C     STORE THREE MUTUALLY PERPENDICULAR                                FFE 1103
C        VECTORS X(I,1), X(I,2), AND X(I,3) GIVEN                       FFE 1104
C        VECTORS U AND V.                                               FFE 1105
      SUBROUTINE AXES(U,V,X)                                            FFE 1106
      DIMENSIONU(3),V(3),X(3,3)                                         FFE 1107
      DO113I#1,3                                                        FFE 1108
  113 X(I,1)#U(I)                                                       FFE 1109
      CALLNORM(U,V,X(1,2))                                              FFE 1110
      CALLNORM(X(1,1),X(1,2),X(1,3))                                    FFE 1111
      RETURN                                                            FFE 1112
      END(0,1,0,0,0)                                                    FFE 1113
*TYPE(FORTRAN)                                                          FFE 1114
C     FIND EIGENVALUES Y OF MATRIX W                                    FFE 1115
      SUBROUTINE EIGVAL(W,Y)                                            FFE 1116
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      COMMONNG                                                          FFE 1117
      DIMENSIONW(3,3),Y(3),X(3),Z(6,6)                                  FFE 1118
      DO119J#1,3                                                        FFE 1119
      DO119I#1,3                                                        FFE 1120
      ZI#W(I,J)                                                         FFE 1121
      Z(I,J)#ZI                                                         FFE 1122
      Z(I+3,J)#ZI                                                       FFE 1123
      Z(I,J+3)#ZI                                                       FFE 1124
  119 Z(I+3,J+3)#ZI                                                     FFE 1125
      P#0.0                                                             FFE 1126
      Q#0.0                                                             FFE 1127
      R#0.0                                                             FFE 1128
      DO207I#1,3                                                        FFE 1129
      P#P-Z(I,I)                                                        FFE 1130
      Q#Q+Z(I,I)*Z(I+1,I+1)-Z(I,I+1)*Z(I+1,I)                           FFE 1131
  207 R#R+Z(3,I)*Z(2,I+1)*Z(1,I+2)-Z(1,I)*Z(2,I+1)*Z(3,I+2)             FFE 1132
      P3#P/3.0                                                          FFE 1133
      A#Q-P*P3                                                          FFE 1134
      B#2.0*P3*P3*P3-Q*P3+R                                             FFE 1135
      B2#B/2.0                                                          FFE 1136
      A3#A/3.0                                                          FFE 1137
      B4#B2*B2                                                          FFE 1138
      A27#A3*A3*A3                                                      FFE 1139
      IF(B4+A27)303,303,215                                             FFE 1140
  215 IF(B4+1.0001*A27)220,220,225                                      FFE 1141
  220 A27#-B4                                                           FFE 1142
      GOTO303                                                           FFE 1143
  225 NG#7                                                              FFE 1144
      GOTO317                                                           FFE 1145
  303 PHI3#(ASINF(SQRTF(1.0+(B4/A27))))/3.0                             FFE 1146
      IF(B)307,305,307                                                  FFE 1147
  305 B#0.0                                                             FFE 1148
  307 C#-SIGNF((2.0*SQRTF(-A3)),B)                                      FFE 1149
      X(1)#C*COSF(PHI3)                                                 FFE 1150
      X(2)#C*COSF(PHI3+4.188790205)                                     FFE 1151
      X(3)#C*COSF(PHI3+2.094395103)                                     FFE 1152
      IF(B)311,313,313                                                  FFE 1153
  311 HOLD#X(1)                                                         FFE 1154
      X(1)#X(3)                                                         FFE 1155
      X(3)#HOLD                                                         FFE 1156
  313 DO315I#1,3                                                        FFE 1157
  315 Y(I)#X(I)-P3                                                      FFE 1158
  317 RETURN                                                            FFE 1159
      END(0,1,0,0,0)                                                    FFE 1160
*TYPE(FORTRAN)                                                          FFE 1161
C     COMPUTE EIGENVECTOR Z OF MATRIX                                   FFE 1162
C        W GIVEN EIGENVALUE Y                                           FFE 1163
      SUBROUTINE EIGVEC(W,Y,Z)                                          FFE 1164
      COMMONNG                                                          FFE 1165
      DIMENSIONW(3,3),X(6,6),Z(3),P(3)                                  FFE 1166
      DO123J#1,3                                                        FFE 1167
      DO123I#1,3                                                        FFE 1168
      XI#W(I,J)                                                         FFE 1169
      X(I,J)#XI                                                         FFE 1170
      X(I+3,J)#XI                                                       FFE 1171
      X(I,J+3)#XI                                                       FFE 1172
  123 X(I+3,J+3)#XI                                                     FFE 1173
      YI#Y                                                              FFE 1174
      DO209I#1,3                                                        FFE 1175
      X(I,I)#X(I,I)-YI                                                  FFE 1176
      X(I+3,I)#X(I+3,I)-YI                                              FFE 1177
      X(I,I+3)#X(I,I+3)-YI                                              FFE 1178
  209 X(I+3,I+3)#X(I+3,I+3)-YI                                          FFE 1179
      SI#0.0                                                            FFE 1180
      DO307I#1,3                                                        FFE 1181
      S#0.0                                                             FFE 1182
      DO223J#1,3                                                        FFE 1183
      PJ#X(I,J+1)*X(I+1,J+2)-X(I,J+2)*X(I+1,J+1)                        FFE 1184
      P(J)#PJ                                                           FFE 1185
  223 S#S+PJ*PJ                                                         FFE 1186
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      IF(S-SI)307,307,301                                               FFE 1187
  301 SI#S                                                              FFE 1188
      DO305J#1,3                                                        FFE 1189
  305 Z(J)#P(J)                                                         FFE 1190
  307 CONTINUE                                                          FFE 1191
      IF(SI)311,311,313                                                 FFE 1192
  311 NG#8                                                              FFE 1193
  313 RETURN                                                            FFE 1194
      END(0,1,0,0,0)                                                    FFE 1195
*TYPE(FORTRAN)                                                          FFE 1196
C     COMPUTE TRACE OF MATRIX X                                         FFE 1197
      FUNCTION TRACE(X)                                                 FFE 1198
      DIMENSIONX(3,3)                                                   FFE 1199
      TRACE#0.0                                                         FFE 1200
      DO111I#1,3                                                        FFE 1201
  111 TRACE#TRACE+X(I,I)                                                FFE 1202
      RETURN                                                            FFE 1203
      END(0,1,0,0,0)                                                    FFE 1204
*TYPE(FORTRAN)                                                          FFE 1205
C     ANGLE SUBROUTINE USED BY FUN2, FUN5, FUN6                         FFE 1206
      FUNCTION FUNA(I)                                                  FFE 1207
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1208
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1209
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1210
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1211
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1212
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1213
      DIMENSIONI(6),X1(3),X2(3),X3(3),V1(3),V2(3)                       FFE 1214
      CALLSTOAA                                                         FFE 1215
      CALLATOM(I(1),X1)                                                 FFE 1216
      CALLATOM(I(3),X2)                                                 FFE 1217
      CALLATOM(I(5),X3)                                                 FFE 1218
      IF(NG)123,117,123                                                 FFE 1219
  117 CALLDIFV(X1,X2,V1)                                                FFE 1220
      CALLDIFV(X3,X2,V2)                                                FFE 1221
      FUNA#ARCCOS(COSVV(V1,V2))                                         FFE 1222
  123 RETURN                                                            FFE 1223
      END(0,1,0,0,0)                                                    FFE 1224
*TYPE(FORTRAN)                                                          FFE 1225
C     DISTANCE SUBROUTINE USED BY FUN1 AND FUN4                         FFE 1226
      FUNCTION FUND(I)                                                  FFE 1227
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1228
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1229
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1230
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1231
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1232
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1233
      DIMENSIONI(4),X1(3),X2(3),V(3)                                    FFE 1234
      CALLSTOAA                                                         FFE 1235
      CALLATOM(I(1),X1)                                                 FFE 1236
      CALLATOM(I(3),X2)                                                 FFE 1237
      CALLDIFV(X2,X1,V)                                                 FFE 1238
      FUND#SQRTF(VMV(V,AA,V))                                           FFE 1239
      RETURN                                                            FFE 1240
      END(0,1,0,0,0)                                                    FFE 1241
*TYPE(FORTRAN)                                                          FFE 1242
C     HEADING 1                                                         FFE 1243
      SUBROUTINE HED1                                                   FFE 1244
      WRITEOUTPUTTAPE9,107                                              FFE 1245
  107 FORMAT(34H0INTERATOMIC DISTANCE IN ANGSTROMS)                     FFE 1246
      RETURN                                                            FFE 1247
      END(0,1,0,0,0)                                                    FFE 1248
*TYPE(FORTRAN)                                                          FFE 1249
C     SET KEY WORDS FOR INTERATOMIC DISTANCE                            FFE 1250
      SUBROUTINE PRE1                                                   FFE 1251
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1252
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1253
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1254
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1255
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1256
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      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1257
      CALLSETKX(IN(2))                                                  FFE 1258
      CALLSETKX(IN(4))                                                  FFE 1259
      RETURN                                                            FFE 1260
      END(0,1,0,0,0)                                                    FFE 1261
*TYPE(FORTRAN)                                                          FFE 1262
C     COMPUTE INTERATOMIC DISTANCE                                      FFE 1263
      SUBROUTINE FUN1                                                   FFE 1264
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1265
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1266
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1267
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1268
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1269
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1270
      FX#FUND(IN(2))                                                    FFE 1271
      RETURN                                                            FFE 1272
      END(0,1,0,0,0)                                                    FFE 1273
*TYPE(FORTRAN)                                                          FFE 1274
C     PUT OUT DESCRIPTION OF INTERATOMIC DISTANCE                       FFE 1275
      SUBROUTINE OUT1                                                   FFE 1276
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1277
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1278
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1279
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1280
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1281
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1282
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,5)                                FFE 1283
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,1H))                 FFE 1284
      RETURN                                                            FFE 1285
      END(0,1,0,0,0)                                                    FFE 1286
*TYPE(FORTRAN)                                                          FFE 1287
C      HEADING 2                                                        FFE 1288
      SUBROUTINE HED2                                                   FFE 1289
      WRITE OUTPUT TAPE 9,107                                           FFE 1290
  107 FORMAT(46H0BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX)         FFE 1291
      RETURN                                                            FFE 1292
      END(0,1,0,0,0)                                                    FFE 1293
*TYPE(FORTRAN)                                                          FFE 1294
C     PRELIMINARY SUBROUTINE 2                                          FFE 1295
      SUBROUTINE PRE2                                                   FFE 1296
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1297
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1298
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1299
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1300
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1301
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1302
      DO107I#2,6,2                                                      FFE 1303
  107 CALLSETKX(IN(I))                                                  FFE 1304
      RETURN                                                            FFE 1305
      END(0,1,0,0,0)                                                    FFE 1306
*TYPE(FORTRAN)                                                          FFE 1307
C     BOND ANGLE SUBROUTINE                                             FFE 1308
      SUBROUTINE FUN2                                                   FFE 1309
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1310
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1311
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1312
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1313
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1314
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1315
      FX#FUNA(IN(2))                                                    FFE 1316
      RETURN                                                            FFE 1317
      END(0,1,0,0,0)                                                    FFE 1318
*TYPE(FORTRAN)                                                          FFE 1319
C     OUTPUT DESCRIPTION 2                                              FFE 1320
      SUBROUTINE OUT2                                                   FFE 1321
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1322
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1323
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1324
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1325
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1326
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      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1327
      WRITE OUTPUT TAPE 9,107,(IN(I),I#2,7)                             FFE 1328
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H))   FFE 1329
      RETURN                                                            FFE 1330
      END(0,1,0,0,0)                                                    FFE 1331
*TYPE(FORTRAN)                                                          FFE 1332
C     HEADING 3                                                         FFE 1333
      SUBROUTINE HED3                                                   FFE 1334
      WRITE OUTPUT TAPE 9,107                                           FFE 1335
  107 FORMAT(58H0DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOFFE 1336
     1MS)                                                               FFE 1337
      RETURN                                                            FFE 1338
      END(0,1,0,0,0)                                                    FFE 1339
*TYPE(FORTRAN)                                                          FFE 1340
C     PRELIMINARY SUBROUTINE 3                                          FFE 1341
      SUBROUTINE PRE3                                                   FFE 1342
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1343
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1344
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1345
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1346
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1347
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1348
      DO107I#2,12,2                                                     FFE 1349
  107 CALLSETKX(IN(I))                                                  FFE 1350
      RETURN                                                            FFE 1351
      END(0,1,0,0,0)                                                    FFE 1352
*TYPE(FORTRAN)                                                          FFE 1353
C     DIHEDRAL ANGLE SUBROUTINE                                         FFE 1354
      SUBROUTINE FUN3                                                   FFE 1355
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1356
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1357
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1358
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1359
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1360
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1361
      DIMENSIONX(3,6),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3)               FFE 1362
      CALLSTOAA                                                         FFE 1363
      CALLSTOBB                                                         FFE 1364
      IF(NG)207,113,207                                                 FFE 1365
  113 DO115I#1,6                                                        FFE 1366
  115 CALLATOM(IN(2*I),X(1,I))                                          FFE 1367
      IF(NG)207,119,207                                                 FFE 1368
  119 CALLDIFV(X(1,2),X(1,1),V1)                                        FFE 1369
      CALLDIFV(X(1,3),X(1,1),V2)                                        FFE 1370
      CALLDIFV(X(1,5),X(1,4),V3)                                        FFE 1371
      CALLDIFV(X(1,6),X(1,4),V4)                                        FFE 1372
      CALLNORM(V1,V2,V5)                                                FFE 1373
      CALLNORM(V3,V4,V6)                                                FFE 1374
      FX#ARCCOS(COSVV(V5,V6))                                           FFE 1375
  207 RETURN                                                            FFE 1376
      END(0,1,0,0,0)                                                    FFE 1377
*TYPE(FORTRAN)                                                          FFE 1378
C     OUTPUT DESCRIPTION 3                                              FFE 1379
      SUBROUTINE OUT3                                                   FFE 1380
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1381
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1382
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1383
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1384
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1385
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1386
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,13)                               FFE 1387
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)/12HFFE 1388
     1          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H))             FFE 1389
      RETURN                                                            FFE 1390
      END(0,1,0,0,0)                                                    FFE 1391
*TYPE(FORTRAN)                                                          FFE 1392
C     HEADING 4                                                         FFE 1393
      SUBROUTINE HED4                                                   FFE 1394
      WRITEOUTPUTTAPE9,107                                              FFE 1395
  107 FORMAT(45H0DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES)          FFE 1396
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      RETURN                                                            FFE 1397
      END(0,1,0,0,0)                                                    FFE 1398
*TYPE(FORTRAN)                                                          FFE 1399
C     PRELIMINARY SUBROUTINE 4                                          FFE 1400
      SUBROUTINE PRE4                                                   FFE 1401
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1402
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1403
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1404
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1405
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1406
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1407
      DO107I#2,9,2                                                      FFE 1408
  107 CALLSETKX(IN(I))                                                  FFE 1409
      RETURN                                                            FFE 1410
      END(0,1,0,0,0)                                                    FFE 1411
*TYPE(FORTRAN)                                                          FFE 1412
C     DIFFERENCE BETWEEN BOND DISTANCES                                 FFE 1413
      SUBROUTINE FUN4                                                   FFE 1414
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1415
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1416
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1417
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1418
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1419
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1420
      FX#FUND(IN(2))-FUND(IN(6))                                        FFE 1421
      RETURN                                                            FFE 1422
      END(0,1,0,0,0)                                                    FFE 1423
*TYPE(FORTRAN)                                                          FFE 1424
C     OUTPUT DESCRIPTION 4                                              FFE 1425
      SUBROUTINE OUT4                                                   FFE 1426
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1427
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1428
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1429
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1430
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1431
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1432
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,9)                                FFE 1433
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,1H)/12H          (12FFE 1434
     1,1H,I3,3H) (I2,1H,I3,1H))                                         FFE 1435
      RETURN                                                            FFE 1436
      END(0,1,0,0,0)                                                    FFE 1437
*TYPE(FORTRAN)                                                          FFE 1438
C     HEADING 5                                                         FFE 1439
      SUBROUTINE HED5                                                   FFE 1440
      WRITEOUTPUTTAPE9,107                                              FFE 1441
  107 FORMAT(35H0DIFFERENCE BETWEEN TWO BOND ANGLES)                    FFE 1442
      RETURN                                                            FFE 1443
      END(0,1,0,0,0)                                                    FFE 1444
*TYPE(FORTRAN)                                                          FFE 1445
C     DIFFERENCE BETWEEN BOND ANGLES                                    FFE 1446
      SUBROUTINE FUN5                                                   FFE 1447
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1448
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1449
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1450
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1451
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1452
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1453
      FX#FUNA(IN(8))-FUNA(IN(2))                                        FFE 1454
      RETURN                                                            FFE 1455
      END(0,1,0,0,0)                                                    FFE 1456
*TYPE(FORTRAN)                                                          FFE 1457
C     HEADING 6                                                         FFE 1458
      SUBROUTINE HED6                                                   FFE 1459
      WRITEOUTPUTTAPE9,107                                              FFE 1460
  107 FORMAT(27H0SUM OF SEVERAL BOND ANGLES)                            FFE 1461
      RETURN                                                            FFE 1462
      END(0,1,0,0,0)                                                    FFE 1463
*TYPE(FORTRAN)                                                          FFE 1464
C     PRELIMINARY SUBROUTINE 6                                          FFE 1465
      SUBROUTINE PRE6                                                   FFE 1466
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      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1467
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1468
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1469
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1470
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1471
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1472
      J#IN(2)*6+1                                                       FFE 1473
      DO109I#3,J,2                                                      FFE 1474
  109 CALLSETKX(IN(I))                                                  FFE 1475
      RETURN                                                            FFE 1476
      END(0,1,0,0,0)                                                    FFE 1477
*TYPE(FORTRAN)                                                          FFE 1478
C     SUM OF BOND ANGLES                                                FFE 1479
      SUBROUTINE FUN6                                                   FFE 1480
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1481
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1482
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1483
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1484
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1485
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1486
      N#IN(2)                                                           FFE 1487
      FX#0.0                                                            FFE 1488
      DO111J#1,N                                                        FFE 1489
  111 FX#FX+FUNA(IN(6*J-3))                                             FFE 1490
      RETURN                                                            FFE 1491
      END(0,1,0,0,0)                                                    FFE 1492
*TYPE(FORTRAN)                                                          FFE 1493
C     OUTPUT DESCRIPTION 6                                              FFE 1494
      SUBROUTINE OUT6                                                   FFE 1495
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1496
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1497
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1498
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1499
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1500
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1501
      J#IN(2)*6+2                                                       FFE 1502
      WRITEOUTPUTTAPE9,109,(IN(I),I#3,J)                                FFE 1503
  109 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)/(12FFE 1504
     1H           (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)))          FFE 1505
      RETURN                                                            FFE 1506
      END(0,1,0,0,0)                                                    FFE 1507
*TYPE(FORTRAN)                                                          FFE 1508
C     SET UP MATRIX AND GET EIGENVALUE                                  FFE 1509
      SUBROUTINE FUNB(W,Z,ZI)                                           FFE 1510
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1511
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1512
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1513
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1514
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1515
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1516
      DIMENSIONB(3,3),W(3,3),Y(3)                                       FFE 1517
      CALLSTOAA                                                         FFE 1518
      CALLBETA(IN(2),B)                                                 FFE 1519
      IF(NG)123,113,123                                                 FFE 1520
  113 CALLMM(B,AA,W)                                                    FFE 1521
      CALLEIGVAL(W,Y)                                                   FFE 1522
      I#IN(4)                                                           FFE 1523
      Z#Y(I)                                                            FFE 1524
      ZI#SQRTF(Z*0.0506605918)                                          FFE 1525
  123 RETURN                                                            FFE 1526
      END(0,1,0,0,0)                                                    FFE 1527
*TYPE(FORTRAN)                                                          FFE 1528
C     COS ANGLE OF PRINCIPAL AXIS AND VECTOR                            FFE 1529
      SUBROUTINE FUNC(C,Z)                                              FFE 1530
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1531
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1532
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1533
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1534
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1535
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1536
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      DIMENSIONW(3,3),X1(3),X2(3),V1(3),V2(3)                           FFE 1537
      CALLFUNB(W,Y,Z)                                                   FFE 1538
      IF(NG)125,111,125                                                 FFE 1539
  111 CALLEIGVEC(W,Y,V1)                                                FFE 1540
      IF(NG)125,115,125                                                 FFE 1541
  115 CALLATOM(IN(5),X1)                                                FFE 1542
      CALLATOM(IN(7),X2)                                                FFE 1543
      IF(NG)125,121,125                                                 FFE 1544
  121 CALLDIFV(X2,X1,V2)                                                FFE 1545
      C#COSVV(V1,V2)                                                    FFE 1546
  125 RETURN                                                            FFE 1547
      END(0,1,0,0,0)                                                    FFE 1548
*TYPE(FORTRAN)                                                          FFE 1549
C     COS ANGLE OF PRINCIPAL AND CARTESIAN AXES                         FFE 1550
      SUBROUTINE FUNX(C,Z)                                              FFE 1551
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1552
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1553
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1554
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1555
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1556
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1557
      DIMENSIONW(3,3),V(3),X(3,4),V1(3),V2(3),AX(3,3)                   FFE 1558
      CALLFUNB(W,Y,Z)                                                   FFE 1559
      CALLSTOBB                                                         FFE 1560
      IF(NG)207,113,207                                                 FFE 1561
  113 CALLEIGVEC(W,Y,V)                                                 FFE 1562
      IF(NG)207,117,207                                                 FFE 1563
  117 DO119I#1,4                                                        FFE 1564
  119 CALLATOM(IN(2*I+4),X(1,I))                                        FFE 1565
      IF(NG)207,123,207                                                 FFE 1566
  123 CALLDIFV(X(1,2),X(1,1),V1)                                        FFE 1567
      CALLDIFV(X(1,4),X(1,3),V2)                                        FFE 1568
      CALLAXES(V1,V2,AX)                                                FFE 1569
      I#IN(5)                                                           FFE 1570
      C#COSVV(V,AX(1,I))                                                FFE 1571
  207 RETURN                                                            FFE 1572
      END(0,1,0,0,0)                                                    FFE 1573
*TYPE(FORTRAN)                                                          FFE 1574
C     HEADING 7                                                         FFE 1575
      SUBROUTINE HED7                                                   FFE 1576
      WRITEOUTPUTTAPE9,107                                              FFE 1577
  107 FORMAT(72HORMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL AFFE 1578
     1XIS R. ANGSTROMS/25H0              ATOM        R)                FFE 1579
      RETURN                                                            FFE 1580
      END(0,1,0,0,0)                                                    FFE 1581
*TYPE(FORTRAN)                                                          FFE 1582
C     PRELIMINARY SUBROUTINE 7                                          FFE 1583
      SUBROUTINE PRE7                                                   FFE 1584
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1585
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1586
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1587
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1588
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1589
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1590
      CALLSETKB(IN(2))                                                  FFE 1591
      RETURN                                                            FFE 1592
      END(0,1,0,0,0)                                                    FFE 1593
*TYPE(FORTRAN)                                                          FFE 1594
C     RMS PRINCIPAL DISPLACEMENT                                        FFE 1595
      SUBROUTINE FUN7                                                   FFE 1596
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1597
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1598
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1599
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1600
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1601
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1602
      DIMENSIONW(3,3)                                                   FFE 1603
      CALLFUNB(W,Z,FX)                                                  FFE 1604
      RETURN                                                            FFE 1605
      END(0,1,0,0,0)                                                    FFE 1606
```

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*TYPE(FORTRAN)
C       OUTPUT DESCRIPTION 7
        SUBROUTINE OUT7
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)
        WRITEOUTPUTTAPE9,107,(IN(I),I#2,4)
  107   FORMAT(12H0                 (I2,1H,I3,6H)        I1)
        RETURN
        END(0,1,0,0,0)
*TYPE(FORTRAN)
C       HEADING 8
        SUBROUTINE HED8
        WRITEOUTPUTTAPE9,107
  107   FORMAT(63H0ANGLE BETWEEN PRINCIPAL AXIS R AND VECTOR DEFINED BY TW
       1O ATOMS/40H0                  ATOM            R            VECTOR)
        RETURN
        END(0,1,0,0,0)
*TYPE(FORTRAN)
C       PRELIMINARY SUBROUTINE 8
        SUBROUTINE PRE8
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)
        CALLSETKB(IN(2))
        DO109I#5,7,2
  109   CALLSETKX(IN(I))
        RETURN
        END(0,1,0,0,0)
*TYPE(FORTRAN)
C       ANGLE BETWEEN PRINCIPAL AXIS AND VECTOR
        SUBROUTINE FUN8
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)
        CALLFUNC(C,Z)
        FX#ARCCOS(C)
        RETURN
        END(0,1,0,0,0)
*TYPE(FORTRAN)
C       OUTPUT DESCRIPTION 8
        SUBROUTINE OUT8
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)
        WRITEOUTPUTTAPE9,107,(IN(I),I#2,8)
  107   FORMAT(12H0               (I2,1H,I3,6H)      I1,5H     (I2,1H,I3,3H) (I2,
       1IH,I3,1H))
        RETURN
        END(0,1,0,0,0)
*TYPE(FORTRAN)
C       HEADING 9
        SUBROUTINE HED9
        WRITEOUTPUTTAPE9,107
  107   FORMAT(113H0RMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL
       1AXIS R PROJECTED ON VECTOR DEFINED BY TWO ATOMS. ANGSTROMS/40H0
       2             ATOM              R               VECTOR)
        RETURN
```

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      END(0,1,0,0,0)                                                    FFE 1677
*TYPE(FORTRAN)                                                          FFE 1678
C     PRINCIPAL AXIS PROJECTED ON VECTOR,                               FFE 1679
      SUBROUTINE FUN9                                                   FFE 1680
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1681
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1682
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1683
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1684
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1685
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1686
      CALLFUNC(C,Z)                                                     FFE 1687
      FX#C*Z                                                            FFE 1688
      RETURN                                                            FFE 1689
      END(0,1,0,0,0)                                                    FFE 1690
*TYPE(FORTRAN)                                                          FFE 1691
C     HEADING 10                                                        FFE 1692
      SUBROUTINE HED10                                                  FFE 1693
      WRITEOUTPUTTAPE9,107                                              FFE 1694
  107 FORMAT(85H0ANGLE BETWEEN PRINCIPAL AXIS R AND AXIS I OF CARTESIAN FFE 1695
     1SYSTEM DEFINED BY TWO VECTORS/45H0              ATOM      R   I   DEFIFFE 1696
     2NING VECTORS)                                                     FFE 1697
      RETURN                                                            FFE 1698
      END(0,1,0,0,0)                                                    FFE 1699
*TYPE(FORTRAN)                                                          FFE 1700
C     PRELIMINARY SUBROUTINE 10                                         FFE 1701
      SUBROUTINE PRE10                                                  FFE 1702
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1703
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1704
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1705
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1706
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1707
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1708
      CALLSETKB(IN(2))                                                  FFE 1709
      DO109I#6,12,2                                                     FFE 1710
  109 CALLSETKX(IN(I))                                                  FFE 1711
      RETURN                                                            FFE 1712
      END(0,1,0,0,0)                                                    FFE 1713
*TYPE(FORTRAN)                                                          FFE 1714
C     ANGLE BETWEEN PRINCIPAL AND CARTESIAN AXES                        FFE 1715
      SUBROUTINE FUN10                                                  FFE 1716
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1717
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1718
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1719
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1720
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1721
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1722
      CALLFUNX(C,Z)                                                     FFE 1723
      FX#ARCCOS(C)                                                      FFE 1724
      RETURN                                                            FFE 1725
      END(0,1,0,0,0)                                                    FFE 1726
*TYPE(FORTRAN)                                                          FFE 1727
C     OUTPUT DESCRIPTION 10                                             FFE 1728
      SUBROUTINE OUT10                                                  FFE 1729
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1730
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1731
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1732
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1733
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1734
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1735
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,13)                               FFE 1736
  107 FORMAT(12H0          (I2,1H,I3,4H)   I1,I3,4H   (I2,1H,I3,3H) (I2,FFE 1737
     1 1H,I3,1H)/30H                              (I2,1H,I3,3H) (I2,1H,I3,FFE 1738
     2 1H))                                                             FFE 1739
      RETURN                                                            FFE 1740
      END(0,1,0,0,0)                                                    FFE 1741
*TYPE(FORTRAN)                                                          FFE 1742
C     HEADING 11                                                        FFE 1743
      SUBROUTINE HED11                                                  FFE 1744
      WRITEOUTPUTTAPE9,107                                              FFE 1745
  107 FORMAT(101H0RMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL FFE 1746
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     1AXIS R PROJECTED ON AXIS I OF CARTESIAN SYSTEM/34H DEFINED BY TWO FFE 1747
     2VECTORS. ANGSTROMS/45H0            ATOM     R  I   DEFINING VECTORFFE 1748
     3S)                                                                FFE 1749
      RETURN                                                            FFE 1750
      END(0,1,0,0,0)                                                    FFE 1751
*TYPE(FORTRAN)                                                          FFE 1752
C     PRINCIPAL AXIS PROJECTED ON CARTESIAN AXIS                        FFE 1753
      SUBROUTINE FUN11                                                  FFE 1754
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1755
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1756
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1757
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1758
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1759
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1760
      CALLFUNX(C,Z)                                                     FFE 1761
      FX#C*Z                                                            FFE 1762
      RETURN                                                            FFE 1763
      END(0,1,0,0,0)                                                    FFE 1764
*TYPE(FORTRAN)                                                          FFE 1765
C     MEAN SQUARE RADIAL DISPLACEMENT                                   FFE 1766
      SUBROUTINE FUNR(I,RSQ)                                            FFE 1767
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1768
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1769
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1770
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1771
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1772
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1773
      DIMENSIONB(3,3),BAA(3,3)                                          FFE 1774
      CALLSTOAA                                                         FFE 1775
      CALLBETA(I,B)                                                     FFE 1776
      CALLMM(B,AA,BAA)                                                  FFE 1777
      RSQ#TRACE(BAA)*0.0506605918                                       FFE 1778
      RETURN                                                            FFE 1779
      END(0,1,0,0,0)                                                    FFE 1780
*TYPE(FORTRAN)                                                          FFE 1781
C     COMPUTE QUANTITIES FOR MEAN BOND DISTANCE                         FFE 1782
      SUBROUTINE FUNCR(C,R)                                             FFE 1783
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1784
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1785
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1786
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1787
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1788
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1789
      DIMENSIONC(2),X(3,2),V(3)                                         FFE 1790
      DO115I#1,2                                                        FFE 1791
      CALLFUNR(IN(2*I),RSQ)                                             FFE 1792
      CALLFUNXI(IN(2*I),IN(2),XISQ)                                     FFE 1793
      C(I)#RSQ-XISQ                                                     FFE 1794
  115 CALLATOM(IN(2*I),X(1,I))                                          FFE 1795
      CALLDIFV(X(1,2),X(1,1),V)                                         FFE 1796
      R#SQRTF(VMV(V,AA,V))                                              FFE 1797
      RETURN                                                            FFE 1798
      END(0,1,0,0,0)                                                    FFE 1799
*TYPE(FORTRAN)                                                          FFE 1800
C     MEAN SQUARE DISPLACEMENT IN GIVEN DIRECTION                       FFE 1801
      SUBROUTINE FUNXI(I,J,XISQ)                                        FFE 1802
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1803
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE 1804
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1805
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1806
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1807
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1808
      DIMENSIONI(2),J(4),B(3,3),X1(3),X2(3),V(3),BAA(3,3),AABAA(3,3)    FFE 1809
      CALLSTOAA                                                         FFE 1810
      CALLBETA(I,B)                                                     FFE 1811
      CALLATOM(J,X1)                                                    FFE 1812
      CALLATOM(J(3),X2)                                                 FFE 1813
      IF(NG)207,117,207                                                 FFE 1814
  117 CALLDIFV(X2,X1,V)                                                 FFE 1815
      D#VMV(V,AA,V)                                                     FFE 1816
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      IF(D)123,123,201                                                  FFE 1817
  123 NG#10                                                             FFE 1818
      GOTO207                                                           FFE 1819
  201 CALLMM(B,AA,BAA)                                                  FFE 1820
      CALLMM(AA,BAA,AABAA)                                              FFE 1821
      XISQ#VMV(V,AABAA,V)*0.0506605918/D                                FFE 1822
  207 RETURN                                                            FFE 1823
      END(0,1,0,0,0)                                                    FFE 1824
*TYPE(FORTRAN)                                                          FFE 1825
C     HEADING 12                                                        FFE 1826
      SUBROUTINE HED12                                                  FFE 1827
      WRITEOUTPUTTAPE9,107                                              FFE 1828
  107 FORMAT(83HORMS COMPONENT OF THERMAL DISPLACEMENT IN DIRECTION DEFIFFE 1829
     1NED BY TWO ATOMS. ANGSTROMS/40H0              ATOM                VFFE 1830
     2ECTOR)                                                            FFE 1831
      RETURN                                                            FFE 1832
      END(0,1,0,0,0)                                                    FFE 1833
*TYPE(FORTRAN)                                                          FFE 1834
C     PRELIMINARY SUBROUTINE 12                                         FFE 1835
      SUBROUTINE PRE12                                                  FFE 1836
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1837
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1838
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1839
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1840
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1841
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1842
      CALLSETKB(IN(2))                                                  FFE 1843
      DO109I#4,6,2                                                      FFE 1844
  109 CALLSETKX(IN(I))                                                  FFE 1845
      RETURN                                                            FFE 1846
      END(0,1,0,0,0)                                                    FFE 1847
*TYPE(FORTRAN)                                                          FFE 1848
C     RMS DISPLACEMENT IN GIVEN DIRECTION                               FFE 1849
      SUBROUTINE FUN12                                                  FFE 1850
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1851
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1852
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1853
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1854
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1855
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1856
      CALLFUNXI(IN(2),IN(4),XISQ)                                       FFE 1857
      FX#SQRTF(XISQ)                                                    FFE 1858
      RETURN                                                            FFE 1859
      END(0,1,0,0,0)                                                    FFE 1860
*TYPE(FORTRAN)                                                          FFE 1861
C     OUTPUT DESCRIPTION 12                                             FFE 1862
      SUBROUTINE OUT12                                                  FFE 1863
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1864
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1865
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1866
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1867
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1868
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1869
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,7)                                FFE 1870
  107 FORMAT(12H0          (I2,1H,I3,12H)          (I2,1H,I3,3H) (I2,1H,FFE 1871
     1I3,1H))                                                           FFE 1872
      RETURN                                                            FFE 1873
      END(0,1,0,0,0)                                                    FFE 1874
*TYPE(FORTRAN)                                                          FFE 1875
C     HEADING 13                                                        FFE 1876
      SUBROUTINE HED13                                                  FFE 1877
      WRITEOUTPUTTAPE9,107                                              FFE 1878
  107 FORMAT(51HORMS RADIAL THERMAL DISPLACEMENT OF ATOM. ANGSTROMS)    FFE 1879
      RETURN                                                            FFE 1880
      END(0,1,0,0,0)                                                    FFE 1881
*TYPE(FORTRAN)                                                          FFE 1882
C     RMS RADIAL DISPLACEMENT                                           FFE 1883
      SUBROUTINE FUN13                                                  FFE 1884
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1885
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1886
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      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1887
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1888
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1889
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1890
      CALLFUNR(IN(2),RSQ)                                               FFE 1891
      FX#SQRTF(RSQ)                                                     FFE 1892
      RETURN                                                            FFE 1893
      END(0,1,0,0,0)                                                    FFE 1894
*TYPE(FORTRAN)                                                          FFE 1895
C     OUTPUT DESCRIPTION 13                                             FFE 1896
      SUBROUTINE OUT13                                                  FFE 1897
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1898
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1899
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1900
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1901
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1902
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1903
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,3)                                FFE 1904
  107 FORMAT(12H0          (I2,1H,I3,1H))                               FFE 1905
      RETURN                                                            FFE 1906
      END(0,1,0,0,0)                                                    FFE 1907
*TYPE(FORTRAN)                                                          FFE 1908
C     HEADING 14                                                        FFE 1909
      SUBROUTINE HED14                                                  FFE 1910
      WRITEOUTPUTTAPE9,107                                              FFE 1911
  107 FORMAT(88H0INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. SECOFFE 1912
     1ND ATOM ASSUMED TO RIDE ON FIRST)                                 FFE 1913
      RETURN                                                            FFE 1914
      END(0,1,0,0,0)                                                    FFE 1915
*TYPE(FORTRAN)                                                          FFE 1916
C     PRELIMINARY SUBROUTINE 14                                         FFE 1917
      SUBROUTINE PRE14                                                  FFE 1918
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1919
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1920
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1921
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1922
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1923
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1924
      DO109I#2,4,2                                                      FFE 1925
      CALLSETKX(IN(I))                                                  FFE 1926
  109 CALLSETKB(IN(I))                                                  FFE 1927
      RETURN                                                            FFE 1928
      END(0,1,0,0,0)                                                    FFE 1929
*TYPE(FORTRAN)                                                          FFE 1930
C     MEAN BOND DISTANCE ASSUMING RIDING                                FFE 1931
      SUBROUTINE FUN14                                                  FFE 1932
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1933
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1934
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1935
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1936
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1937
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1938
      DIMENSIONC(2)                                                     FFE 1939
      CALLFUNCR(C,R)                                                    FFE 1940
      FX#R+(C(2)-C(1))/(2.0*R)                                          FFE 1941
      RETURN                                                            FFE 1942
      END(0,1,0,0,0)                                                    FFE 1943
*TYPE(FORTRAN)                                                          FFE 1944
C     HEADING 15                                                        FFE 1945
      SUBROUTINE HED15                                                  FFE 1946
      WRITEOUTPUTTAPE9,107                                              FFE 1947
  107 FORMAT(87H0INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. ATOMFFE 1948
     1S ASSUMED TO MOVE INDEPENDENTLY)                                  FFE 1949
      RETURN                                                            FFE 1950
      END(0,1,0,0,0)                                                    FFE 1951
*TYPE(FORTRAN)                                                          FFE 1952
C     MEAN INTERATOMIC DISTANCE ASSUMING INDEPENDENT MOTION             FFE 1953
      SUBROUTINE FUN15                                                  FFE 1954
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1955
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1956
```

```
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1957
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1958
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1959
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1960
      DIMENSIONC(2)                                                     FFE 1961
      CALLFUNCR(C,R)                                                    FFE 1962
      FX#R+(C(2)+C(1))/(2.0*R)                                          FFE 1963
      RETURN                                                            FFE 1964
      END(0,1,0,0,0)                                                    FFE 1965
*TYPE(FORTRAN)                                                          FFE 1966
C     DUMMY SUBROUTINE. MAY BE CHANGED BY USER.                         FFE 1967
      SUBROUTINE SETA(A)                                                FFE 1968
      RETURN                                                            FFE 1969
      END(0,1,0,0,0)                                                    FFE 1970
*TYPE(FORTRAN)                                                          FFE 1971
C     DUMMY SUBROUTINE. MAY BE CHANGED BY USER.                         FFE 1972
      SUBROUTINE SETP(P)                                                FFE 1973
      RETURN                                                            FFE 1974
      END(0,1,0,0,0)                                                    FFE 1975
```

SUBROUTINES FOR EXAMPLES

```
*TYPE(FORTRAN)                                                          FFE 1976
C     EXAMPLES 1 AND 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.     FFE 1977
      SUBROUTINE SETA(A)                                                FFE 1978
      DIMENSION A(6)                                                    FFE 1979
      A(2)#A(1)                                                         FFE 1980
      RETURN                                                            FFE 1981
      END(0,1,0,0,0)                                                    FFE 1982
*TYPE(FORTRAN)                                                          FFE 1983
C     EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.            FFE 1984
      SUBROUTINE SETP(P)                                                FFE 1985
      DIMENSION P(100)                                                  FFE 1986
      P(5)#P(4)                                                         FFE 1987
      RETURN                                                            FFE 1988
      END(0,1,0,0,0)                                                    FFE 1989
*TYPE(FORTRAN)                                                          FFE 1990
C     EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.            FFE 1991
      SUBROUTINE SETP(P)                                                FFE 1992
      DIMENSION P(100)                                                  FFE 1993
      P(17)#P(16)                                                       FFE 1994
      P(20)#P(19)                                                       FFE 1995
      P(24)#-P(23)                                                      FFE 1996
      RETURN                                                            FFE 1997
      END(0,1,0,0,0)                                                    FFE 1998
```

DATA FOR EXAMPLES

```
*DATA                                                                   FFE 1999
EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT. FFE 2000
  1  6  1  5  4  3  1  0  0                                              FFE 2001
 .4155727 .2676554 .1179998 .5294765 .5294765 .3333333                  FFE 2002
111100                                                                  FFE 2003
         1.0                                                            FFE 2004
 .85384856-7 .73725640-7-.29955735-7-.68440656-8 .13675298-6-.57040983-7FFE 2005
 .11775529-7 .97987015-7 .20795807-7 .33845897-7                        FFE 2006
    4.913        0     5.404        0        0      -0.5               FFE 2007
     .005        0      .010        0        0                         FFE 2008
            1-2            -2            -3                             FFE 2009
            2-1            -1     .33333333+3                           FFE 2010
            1               2-1   .33333333-3                           FFE 2011
```

```
            2                 1-2  .66666667+3                          FFE 2012
            2                 1    .66666667-3                          FFE 2013
  1  2300  1  2                                                          FFE 2014
  1  2300  1300                                                          FFE 2015
  2  1  2  2300  1  3                                                    FFE 2016
  2  1300  2300  1305                                                    FFE 2017
  2  1300  2300  1  2                                                    FFE 2018
  3  2300  1  2  1  3  2300  1300  1305                                  FFE 2019
  4  2300  1  2  2300  1300                                              FFE 2020
  5  1  2  2300  1  3  1300  2300  1305                                  FFE 2021
  0                                                                     FFE 2022
*DATA                                                                   FFE 2023
EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.FFE 2024
  1  0  1  5                                                            FFE 2025
    4.913        0    5.404        0        0     -0.5                  FFE 2026
     .005        0     .010        0        0                          FFE 2027
            1-2            -2             -3                            FFE 2028
            2-1            -1    .33333333+3                            FFE 2029
            1               2-1  .33333333-3                            FFE 2030
            2               1-2  .66666667+3                            FFE 2031
            2               1    .66666667-3                            FFE 2032
  1  2300  1  2                                                          FFE 2033
  1  2300  1300                                                          FFE 2034
  2  1  2  2300  1  3                                                    FFE 2035
  2  1300  2300  1305                                                    FFE 2036
  2  1300  2300  1  2                                                    FFE 2037
  3  2300  1  2  1  3  2300  1300  1305                                  FFE 2038
  4  2300  1  2  2300  1300                                              FFE 2039
  5  1  2  2300  1  3  1300  2300  1305                                  FFE 2040
207  2  0                                                               FFE 2041
108  1  2     2300  1  2                                                 FFE 2042
110  1  2        2300  1  2  2300  1  3                                  FFE 2043
110  2300        2300  2  0  2300  2700                                  FFE 2044
 12  1  2  2300  1  2                                                    FFE 2045
 12  2300  2300  1  2                                                    FFE 2046
 13  1  2                                                               FFE 2047
 13  2300                                                               FFE 2048
 15  2300  1  2                                                          FFE 2049
  0                                                                     FFE 2050


*TYPE(BINARY)                                                           FFE 2051
```

PROGRAM OUTPUT FOR EXAMPLES

```
EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT.

INPUT DATA TO BE READ FROM CARDS

NUMBER OF STRUCTURE PARAMETERS IS   6

VARIANCE-COVARIANCE MATRIX AND PARAMETER SELECTION INFORMATION WILL
BE USED

NUMBER OF SYMMETRY CARDS IS  5

CELL PARAMETER ERRORS ARE
TO BE READ IN THE FORM OF STANDARD ERRORS

ORDER OF THE VARIANCE-COVARIANCE MATRIX FOR THE STRUCTURE PARAMETERS IS  4

PERIOD OF THE POSITION PARAMETERS IN THE PARAMETER LIST IS  3

POSITION OF THE FIRST X COORDINATE IN THE PARAMETER LIST IS  1

INPUT DATA

  I      P(I)  KI1(I)

  1     0.4156   1
  2     0.2677   1
  3     0.1180   1
  4     0.5295   1
  5     0.5295   0
  6     0.3333   0


EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT.

CELL PARAMETERS

     4.9130     0.         5.4040     0.         0.        -0.5000

STANDARD ERRORS, RESPECTIVELY, OF THE ABOVE CELL PARAMETERS

     0.0050     0.         0.0100     0.         0.         0.

SYMMETRY INFORMATION

     TRANSFORMED X           TRANSFORMED Y           TRANSFORMED Z

    -0.       1-2           -0.       -2-0          -0.       -3-0
    -0.       2-1           -0.       -1-0           0.333333 3-0
    -0.      -1-0           -0.        2-1           0.333333-3-0
    -0.      -2-0           -0.        1-2           0.666667 3-0
    -0.       2-0           -0.        1-0           0.666667-3-0


EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT.


INTERATOMIC DISTANCE IN ANGSTROMS

              ( 2,300) ( 1,  2)
                                                  1.6012 +OR- 0.0019 ( 0.0012)

              ( 2,300) ( 1,300)
                                                  1.6131 +OR- 0.0021 ( 0.0012)
```

```
BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX

          ( 1,  2) ( 2,300) ( 1,  3)
                                                109.2048 +OR- 0.1013 ( 0.0975)

          ( 1,300) ( 2,300) ( 1,305)
                                                110.1962 +OR- 0.1689 ( 0.1443)

          ( 1,300) ( 2,300) ( 1,  2)
                                                109.9518 +OR- 0.0875 ( 0.0755)

DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOMS

          ( 2,300) ( 1,  2) ( 1,  3)
          ( 2,300) ( 1,300) ( 1,305)
                                                 89.1600 +OR- 0.1128 ( 0.0478)

DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES

          ( 2,300) ( 1,  2)
          ( 2,300) ( 1,300)
                                                -0.0119 +OR- 0.0026 ( 0.0022)

DIFFERENCE BETWEEN TWO BOND ANGLES

          ( 1,  2) ( 2,300) ( 1,  3)
          ( 1,300) ( 2,300) ( 1,305)
                                                  0.9914 +OR- 0.1787 ( 0.1681)


EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.

INPUT DATA TO BE READ FROM OR FLS TAPE

VARIANCE-COVARIANCE MATRIX AND PARAMETER SELECTION INFORMATION WILL
BE USED

NUMBER OF SYMMETRY CARDS IS  5

CELL PARAMETER ERRORS ARE
TO BE READ IN THE FORM OF STANDARD ERRORS

NUMBER OF STRUCTURE PARAMETERS IS  24

PERIOD OF THE POSITION PARAMETERS IN THE PARAMETER LIST IS 11

POSITION OF THE FIRST X COORDINATE IN THE PARAMETER LIST IS  5

PERIOD OF THE TEMPERATURE FACTOR COEFFICIENTS IN THE PARAMETER LIST IS 11

POSITION OF THE FIRST TEMPERATURE FACTOR COEFFICIENT IN THE PARAMETER LIST IS  8

ORDER OF THE VARIANCE-COVARIANCE MATRIX FOR THE STRUCTURE PARAMETERS IS 15

INPUT DATA

  I      P(I)   KII(I)

  1     1.0004    1
  2     0.        0
  3     1.0000    0
  4     1.0000    0
  5     0.4156    1
  6     0.2677    1
  7     0.1180    1
  8     0.0039    1
  9     0.0045    1
 10     0.0027    1
```

11	0.0020	1
12	0.0000	1
13	0.0002	1
14	2.0000	0
15	0.5000	0
16	0.5295	1
17	0.5295	0
18	0.3333	0
19	0.0067	1
20	0.0067	0
21	0.0040	1
22	0.0034	1
23	0.0002	1
24	-0.0002	0

EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.

CELL PARAMETERS

4.9130	0.	5.4040	0.	0.	-0.5000

STANDARD ERRORS, RESPECTIVELY, OF THE ABOVE CELL PARAMETERS

0.0050	0.	0.0100	0.	0.	0.

SYMMETRY INFORMATION

TRANSFORMED X		TRANSFORMED Y		TRANSFORMED Z	
-0.	1-2	-0.	-2-0	-0.	-3-0
-0.	2-1	-0.	-1-0	0.333333	3-0
-0.	-1-0	-0.	2-1	0.333333	-3-0
-0.	-2-0	-0.	1-2	0.666667	3-0
-0.	2-0	-0.	1-0	0.666667	-3-0

EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.

INTERATOMIC DISTANCE IN ANGSTROMS

(2,300) (1, 2)
1.6012 +OR- 0.0019 (0.0012)

(2,300) (1,300)
1.6131 +OR- 0.0021 (0.0012)

BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX

(1, 2) (2,300) (1, 3)
109.2048 +OR- 0.1014 (0.0977)

(1,300) (2,300) (1,305)
110.1962 +OR- 0.1688 (0.1441)

(1,300) (2,300) (1, 2)
109.9518 +OR- 0.0875 (0.0756)

DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOMS

(2,300) (1, 2) (1, 3)
(2,300) (1,300) (1,305)
89.1600 +OR- 0.1128 (0.0477)

DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES

(2,300) (1, 2)
(2,300) (1,300)
-0.0119 +OR- 0.0026 (0.0022)

DIFFERENCE BETWEEN TWO BOND ANGLES

```
( 1,  2) ( 2,300) ( 1,  3)
( 1,300) ( 2,300) ( 1,305)
                                        0.9914 +OR- 0.1784 ( 0.1679)
```

RMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL AXIS R. ANGSTROMS

```
  ATOM        R

( 1,  0)      1
                                        0.0600 +OR- 0.0073 ( 0.0073)

( 1,  0)      2
                                        0.0619 +OR- 0.0050 ( 0.0050)

( 1,  0)      3
                                        0.0668 +OR- 0.0068 ( 0.0068)

( 2,  0)      1
                                        0.0742 +OR- 0.0033 ( 0.0033)

( 2,  0)      2
                                        0.0785 +OR- 0.0033 ( 0.0033)

( 2,  0)      3
                                        0.0798 +OR- 0.0035 ( 0.0035)
```

ANGLE BETWEEN PRINCIPAL AXIS R AND VECTOR DEFINED BY TWO ATOMS

```
  ATOM        R          VECTOR

( 1,  2)      1    ( 2,300) ( 1,  2)
                                       76.6802 +OR-56.4312 (56.4311)

( 1,  2)      2    ( 2,300) ( 1,  2)
                                       79.0386 +OR-57.5388 (57.5340)

( 1,  2)      3    ( 2,300) ( 1,  2)
                                       17.3808 +OR-39.1984 (39.1957)
```

ANGLE BETWEEN PRINCIPAL AXIS R AND AXIS I OF CARTESIAN SYSTEM DEFINED BY TWO VECTORS

```
  ATOM      R  I   DEFINING VECTORS

( 1,  2)    1  1   ( 2,300) ( 1,  2)
                   ( 2,300) ( 1,  3)
                                       76.6802 +OR-56.4312 (56.4311)

( 1,  2)    1  2   ( 2,300) ( 1,  2)
                   ( 2,300) ( 1,  3)
                                       77.3633 +OR-51.2667 (51.2667)

( 1,  2)    1  3   ( 2,300) ( 1,  2)
                   ( 2,300) ( 1,  3)
                                      161.4757 +OR-80.2633 (80.2633)

( 1,  2)    2  1   ( 2,300) ( 1,  2)
                   ( 2,300) ( 1,  3)
                                       79.0386 +OR-57.5388 (57.5340)

( 1,  2)    2  2   ( 2,300) ( 1,  2)
                   ( 2,300) ( 1,  3)
                                      164.9587 +OR-32.7963 (32.7957)

( 1,  2)    2  3   ( 2,300) ( 1,  2)
                   ( 2,300) ( 1,  3)
                                      100.1726 +OR-48.7792 (48.7790)
```

```
( 1,  2)   3  1   ( 2,300) ( 1,  2)
                  ( 2,300) ( 1,  3)
                                        17.3808 +OR-39.1984 (39.1957)

( 1,  2)   3  2   ( 2,300) ( 1,  2)
                  ( 2,300) ( 1,  3)
                                        81.9750 +OR-43.5891 (43.5834)

( 1,  2)   3  3   ( 2,300) ( 1,  2)
                  ( 2,300) ( 1,  3)
                                        74.6870 +OR-37.9786 (37.9784)

( 2,300)   1  1   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        90.0000 +OR- 0.     ( 0.    )

( 2,300)   1  2   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        45.2094 +OR-24.2878 (24.2720)

( 2,300)   1  3   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        44.7906 +OR-24.2879 (24.2721)

( 2,300)   2  1   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                       179.9815 +OR- 1.4866 ( 1.3871)

( 2,300)   2  2   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        89.9902 +OR- 3.0562 ( 2.6073)

( 2,300)   2  3   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        90.0183 +OR- 5.7403 ( 4.8985)

( 2,300)   3  1   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        90.0000 +OR- 0.     ( 0.    )

( 2,300)   3  2   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                       135.2073 +OR-24.0921 (24.0671)

( 2,300)   3  3   ( 2,300) ( 2,  0)
                  ( 2,300) ( 2,700)
                                        45.2073 +OR-24.0921 (24.0672)
```

RMS COMPONENT OF THERMAL DISPLACEMENT IN DIRECTION DEFINED BY TWO ATOMS. ANGSTROMS

```
        ATOM                VECTOR

( 1,  2)            ( 2,300) ( 1,  2)
                                        0.0662 +OR- 0.0067 ( 0.0067)

( 2,300)            ( 2,300) ( 1,  2)
                                        0.0791 +OR- 0.0022 ( 0.0022)
```

RMS RADIAL THERMAL DISPLACEMENT OF ATOM. ANGSTROMS

```
( 1,  2)
                                        0.1090 +OR- 0.0036 ( 0.0036)

( 2,300)
                                        0.1343 +OR- 0.0016 ( 0.0016)
```

INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. ATOMS ASSUMED TO MOVE INDEPENDENTLY

```
( 2,300) ( 1,  2)
                                        1.6072 +OR- 0.0019 ( 0.0012)
```

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A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Carroll K. Johnson

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Carroll K. Johnson

JUNE 1965

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OR TEP: A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

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ABSTRACT

This report describes a computer program for drawing crystal structure illustrations with a mechanical plotter. Ball-and-stick type illustrations of a quality suitable for publication are produced with either spheres or thermal-motion probability ellipsoids on the atomic sites. The program can produce stereoscopic pairs of illustrations which aid in the visualization of complex packing arrangements of atoms and thermal motion patterns. Interatomic distances, bond angles, and principal axes of thermal motion are also calculated to aid the structural study.

The FORTRAN coding utilizes the comparable features of IBM 709/7090 FORTRAN II and CDC 1604/1604A FORTRAN 63 so that the program can be executed on a number of different machines which have 32 K word memories. The machine-oriented plotting subroutines are standard library-type routines with slight modifications. Both CalComp and Benson Lehner off-line magnetic-tape plotting systems have been used successfully.

Sample stereo-figure illustrations and a viewer are included with the report.

1. INTRODUCTION

Appropriate illustrations are essential in any manuscript dealing with crystallographic structures. An often quoted expression might justifiably be paraphrased to read that a well-planned figure is worth a thousand numbers. With the so-called information explosion in its early exponential stages, the author of a structure paper should feel particularly obligated to help the reader as much as he can with "crystal clear" illustrations.

This computer program, OR TEP (Oak Ridge Thermal Ellipsoid Plot program) is an attempt to supply a tool which can reduce the tedium associated with drawing certain types of crystal structure illustrations. In addition, the precision obtainable through machine plotting makes feasible the production of detailed stereoscopic illustrations which are impractical to draw by conventional drafting methods. The program does not in any sense replace the experience of the crystallographic draftsman; it is only a way of implementing certain of his ideas. Touching up the figures by hand to correct for overlap and to add further detail greatly enhances the figure's appeal and usefulness. The user is encouraged to do this and not to be content with the raw illustrations as they come from the plotter.

Four major goals were specified for OR TEP, and they are listed here in the order of their assigned importance. (1) The program must produce high quality illustrations, including stereoscopic pairs of thermal-motion figures, as free as possible of visually distracting approximations. (2) The program must be general both with respect to the types of illustrations it can draw and the types of computing and plotting equipment that it can utilize. (3) The program must be easy to use and require a minimum of input; it should also be easy to modify. (4) The computation time should be minimized. Memory size limitation was not one of the considerations; hence the program requires a 32 K word memory.

Stereoscopic crystal structure illustrations were used quite extensively in the 1920's and 1930's, particularly by M. von Laue and R. von Mises in their beautifully done two-volume series of stereoscopic drawings.[1] More recently, computer techniques were applied in making crystal structure stereoscopic pictures by W. R. Busing[2] using an IBM 704 computer with cathode ray tube output. The availability of larger, faster computers and higher resolution plotting devices led quite naturally to the present work. As usual, there is an unlimited horizon for future work with more sophisticated ideas and equipment.

I am particularly indebted to my colleagues, Drs. H. A. Levy, W. R. Busing, G. M. Brown, and R. D. Ellison, for many helpful discussions, and to R. A. Hollister, a summer participant with the ORNL Mathematics Division, who helped plan and code several parts of the program. The initial version of OR TEP was written as a subroutine for the Busing, Martin, and Levy Function and Error Program, OR FFE;[3] and many of the concepts and several of the subroutines of OR FFE are incorporated into the present program. Several parts of EIGEN were taken from a program written by R. E. Funderlic and B. Franz from the Central Data Processing group. Subroutine AXEQB was adapted from a subroutine obtained from the Oak Ridge Central Data Processing Library.

This report covers the following topics. First, Sect. 2.1 is a summary table of instructions and is the part of the report to which the experienced user will routinely refer. Next, the philosophy of the program is outlined and an example given. Section 3 defines the terms used in this report and describes the input in detail. The computational procedures used by the program are discussed in Sect. 4, and steps are outlined for adapting the program to other configurations of equipment. The next section summarizes the mathematics of thermal motion probability ellipsoids. Section 6 contains a number of examples of figures produced with OR TEP. Most of these drawings are stereoscopic pairs of perspective projections and are included to illustrate the information transfer advantages gained through the use of stereo figures. The final section contains the complete OR TEP FORTRAN listing.

2. GENERAL PRINCIPLES AND PROCEDURES

2.1 Summary Table of Instructions

A brief summary of the input cards is given at this point to serve as a check list for use with OR TEP. All aspects are explained in detail in Sect. 3.

1. *Title card* (see 3.2.1)
2. *Cell parameter card* (see 3.2.2)
3. *Symmetry cards* with sentinel in column 1 on last card (see 3.2.3)
4. *Atomic parameter cards* (two per atom) with sentinel in column 1 of very last card (see 3.2.4)
5. *Instruction cards* with -1 in columns 8 and 9 of final instruction card. The instructions are summarized in Table 2.1 and explained in detail in Sect. 3.3.

---

[1] M. von Laue and R. von Mises (eds.), *Stereoscopic Drawings of Crystal Structures*, vols. I and II, Springer, Berlin, 1926 and 1936.

[2] W. R. Busing, *Abstract of Washington, D.C., Meeting of the ACA, Jan. 24–27, 1960*, F-7, p. 23.

[3] W. R. Busing, K. O. Martin, and H. A. Levy, *OR FFE, a FORTRAN Crystallographic Function and Error Program*, ORNL-TM-306 (March 1964).

Table 2.1. Summary Table of All Instructions

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Structure analysis									
Distances	0 or 2	101	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Dist. + ang.	0 or 2	102	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Princ. axes	–	103	–	–	–	–	–	–	–
Plotter control									
Initialize	–	201	–	–	–	–	–	–	–
Advance and term.	–	202	X(IN)	Y(IN)	–	–	–	–	–
Plot boundary									
Dimensions	–	301	X(IN)	Y(IN)	VIEW(IN)	BRDR(IN)	–	–	–
Title rotation	–	302	THETA (°)	–	–	–	–	–	–
Retrace displace	–	303	X(IN)	–	–	–	–	–	–
Atoms list									
Run add	–	401	From	(–) to	From	(–) to	....	....	....
Run subtract	–	411	From	(–) to	From	(–) to	....	....	....
Sphere add	0 or 2	402	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Sphere subtract	0 or 2	412	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Box add	–	403	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Box subtract	–	413	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Zero atoms list	–	410	–	–	–	–	–	–	–
Cartesian system									
Definition	–	501	ORGN	V1A	V1B	V2A	V2B	–	–
Rotate reference	–	502	Axes No.	Rotate (°)	Axes No.	Rotate (°)	....	....	....
Rotate working	–	503	Axes No.	Rotate (°)	–	–	–	–	–

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Center and scale									
Explicit	–	601	XO (IN)	YO (IN)	SCAL1	SCAL2	–	–	–
Scale only	–	602	XO (IN)	YO (IN)	–	SCAL2	–	–	–
Center only	–	603	–	–	SCAL1	SCAL2	–	–	–
Center and scale	–	604	–	–	–	SCAL2	–	–	–
I. P. and I. S.[a]	–	611	ΔXO (IN)	ΔYO (IN)	ΔSCAL1	SCAL2	–	–	–
I. P. and scale	–	612	ΔXO (IN)	ΔYO (IN)	–	SCAL2	–	–	–
I. S. and center	–	613	–	–	ΔSCAL1	SCAL2	–	–	–
Ellipsoids									
Shaded football	0 or 1	701	–	–	–	–	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)	–	–	A0 (IN)	A1 (IN)	–	–	–	–	–
Football	0 or 1	702	(same as 701)						
Open model	0 or 1	703	(same as 701)						
Boundary only	0 or 1	704	(same as 701)						
Other types	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)	–		A0 (IN)	A1 (IN)					
As above except no	0 or 1	711	(same as 701)						
printed output of	0 or 1	712	(same as 701)						
individual coordinates	0 or 1	713	(same as 701)						
	0 or 1	714	(same as 701)						
	0 or 1	715	(same as 705)						
Bonds									
Explicit (cont.)	0 or 1	801	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	....
Implicit fancy (Format No. 2 trailer card)	2	802	–	–	–	–	–	–	–
Implicit line (Format No. 2 trailer card)	2	803	–	–	–	–	–	–	–

[a]I. P. and I. S. signifies increment position and increment scale.
[b]PAR-OFF signifies parallel offset (in.).
[c]PER-OFF signifies perpendicular offset (in.).

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
As above except	–	811	(same as 801)						
no printed output	2	812	(same as 802)						
	2	813	(same as 803)						
Labels									
CHEM SYMB	–	901	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
REG TITLES	3	902	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3									
title card									
PROJ VECT TITLE	3	903	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3									
title card									
VECTOR TITLE	3	913	ATOM-1	ATOM-2	–	–	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3									
title card									
PROJ BOND LABEL	–	904	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(1, 2, 3 dec. places)	–	905							
	–	906							
BOND LABEL	–	914	ATOM-1	ATOM-2	–	–	HGT (IN)	PAR-OFF	PER-OFF
(1, 2, 3 dec. places)	–	915							
	–	916							
CENTERED SYMB		908	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(with pen up or pen down)	1	909							
(Format No. 1 trailer card)	1	–	SYMB#	–	–	–	–	–	–
Saved sequence	–								
START	–	1101	–	–	–	–	–	–	–
STOP	–	1102	–	–	–	–	–	–	–
EXECUTE	–	1103	–	–	–	–	–	–	–
Terminate job	–	–1	–	–	–	–	–	–	–
New job follows (from title card on)	–	–2	–	–	–	–	–	–	–

2.2 Programming a Nonstereoscopic Illustration for OR TEP

2.2.1 General Comments on Automated Graphics. – In order to produce high quality illustrations with OR TEP, one must in general use an iterative approach; that is, the illustration must usually be computed and plotted several times before an optimal figure is produced. With each trial, as many factors as possible are optimized to give a more informative and more esthetically pleasing result. One often requires about four trials for a stereoscopic figure of an unfamiliar structure (barring blunders and plotter malfunctions).

Overlap is one of the major problems, particularly for chemical symbols and bond distance labels. If the user is not drawing stereoscopic figures, it is often better to do the lettering with a LeRoy lettering template instead of the computer. The template lettering is neater than the computer lettering, and it can be positioned much more easily. However, for stereoscopic lettering the manual procedure appears to be unsatisfactory because of the necessity for exact relative placement of the lettering on the two views to maintain good stereopsis.

Overlapping atoms are another problem. The program does not leave out the parts of an atom hidden behind other atoms. This feature would be a difficult (although not impossible) programming feat. This can be accomplished manually, however, by erasing or "whiting out" the unwanted parts of an atom. Even with stereo views, the figures are more effective if overlap is taken care of, especially when "opaque" ellipsoids are used.

In order to maintain generality in OR TEP, the concept of programming is applied to the problem of drawing illustrations with a plotter. This concept allows access to a series of basic building block operations which are put together by the user to "program" an illustration. The instructions used in programming OR TEP are divided into the following categories: (1) instructions used to specify preliminary graphical details, (2) instructions used to compose an illustration, (3) instructions used to draw the illustration, (4) instructions used to repeat a sequence of other instructions, and (5) termination instructions. Each instruction starts on a separate punched card and contains an identifying number and whatever parameters are needed for the particular instruction. The general role of these instructions is explained in the remaining sections of Part 2, and the individual instructions are described in detail in 3.3. The simplest way to construct the program is, first, to scan through the list of instructions in numerical order and pick out the relevant ones to construct the framework of the program. Then certain other instructions are placed into the framework program to furnish the remaining "bookkeeping" details.

Let us assume that the structural data cards (described in 3.2) have been prepared for a crystal structure and that we want to prepare a program to draw a single nonstereographic figure of the contents of one unit cell. We describe next the general stepwise procedure one would follow to program such an illustration.

2.2.2 Preliminary Graphical Details. – The first instruction card should be the plotter control instruction 201 (see 3.3.3.1) which will initialize the plotting package.

Next, the plot boundary instruction 301 (see 3.3.4.1) is needed to set the following parameters: (1) X dimension in inches for the plot boundary, (2) Y dimension in inches for the plot boundary, (3) viewing

distance in inches for perspective projection (zero as a signal for parallel projection), and (4) border (or margin) dimension inside the boundary.

No other 200 or 300 series instructions are required for this particular hypothetical figure.

The preliminary graphical details are analogous to what a draftsman might do in setting up his drafting board in preparation for a drawing.

2.2.3 Composing the Illustration. – This step involves specifying: (1) which atoms are to be used as the figure subject, (2) the rotational orientation of the subject, and (3) the scaling and positioning of the subject relative to the drawing area. These three components of composition are implemented by the 400, 500, and 600 series instructions respectively.

For our hypothetical example, suppose we want to place the *b* crystal axis along the plotter *x* axis and the c axis of the crystal in the plotter *xy* plane as nearly as possible parallel to the plotter *y* axis. This setting can be accomplished with a 501 instruction (see 3.3.6.1) alone; but if additional reorientation were necessary, a 502 instruction (see 3.3.6.2) would also be used.

A rectangular box of enclosure can be described with a 403 instruction (see 3.3.5.3) to contain the desired atoms for the subject definition. The scaling and positioning of the subject to fill the drawing area may be accomplished automatically with a 604 instruction (see 3.3.7.1).

2.2.4 Drawing the Illustration. – Crystal structure illustrations of the ball-and-stick type are made up of three components: balls (atoms), sticks (bonds), and labels. The three components are drawn with the 700, 800, and 900 instruction series respectively; the first two instruction series can also perform certain types of labeling.

The atom representation can be either a general ellipsoid or a boundary ellipse. In some cases these become a sphere and a circle. Chemical symbols may be plotted simultaneously with the atoms.

For our example we might simply draw circles and put the chemical symbols within the circles by using instruction 704 (see 3.3.8.1). This instruction will draw all the atoms of the subject and their chemical symbols.

The bonds are not always necessary in a drawing, but for structures with molecules or with distinctive groupings they are usually quite helpful. The most convenient method for describing and drawing bonds is instruction 812 (see 3.3.9.2). This instruction uses vector search codes (see 3.1.5) which reflect the user's knowledge of the structural chemistry and the interatomic distance ranges for the compound being drawn. Covalent bonds or any other desired type are found and drawn automatically from the list of atoms which make up the subject. If desired, the interatomic distance label can also be drawn with each bond (see 3.3.9).

Various types of labeling can be done with the 900 series instruction. The one which will most often be included is a caption for the figure using instruction 902 (see 3.3.10.2).

2.2.5 Terminating the Drawing of the Illustration. – The plotter control instruction 202 (see 3.3.3.2) allows the user to remove the finished drawing from the plotting area and to place a fresh area of plot paper in position for any additional plots which may be drawn.

To terminate the computer job, a (−1) instruction (see 3.3.12) would be used as the last instruction of the program.

2.3 Programming a Stereoscopic Illustration for OR TEP

A stereoscopic pair of figures is simply two perspective views of the subject as seen from two different viewpoints (which are usually about 6° apart). This pair is produced with OR TEP by programming for two drawings. A few additional instructions supplementary to those outlined in 2.2 are useful for producing stereo figures. These instructions are the stereoscopic rotation instruction 503 and the 1100 series of instructions, which facilitate the repetition of a series of instructions.

2.3.1 Stereoscopic Rotations. – In general, one member of a detailed stereoscopic illustration cannot be drawn completely independent of the other member of the pair because certain features (e.g., which octant of an ellipsoid is shaded) must be done identically in the two drawings. In OR TEP the "stereoscopically sensitive decisions" are handled by using two Cartesian coordinate systems: the reference Cartesian system and the working Cartesian system (see 3.1.8). The steps involved in picture composition (see 2.2.3) and the stereoscopically sensitive decisions are always based on the reference system, but the drawing of the illustration (see 2.2.4) is always based on the working system. A stereoscopic rotation is simply a rotation of the working system *from the reference system* about the axis which is vertical while viewing the final result. For example, a nominal rotation of +3° about the plotter *y* axis might be used for the left-eye view and a rotation of −3° about the same axis might be made before plotting the right-eye view, thus producing a total interocular angle of 6°.

A program to draw a stereo pair would involve the following steps:

1. preliminary graphical details,
2. composition of subject,
3. left-eye stereo rotation,
4. draw the subject,
5. advance the plotter,
6. right-eye stereo rotation,
7. draw the subject,
8. advance the plotter,
9. terminate the job.

2.3.2 Repeating a Sequence of Operations. – It should be noted that steps 7 and 8 in the stereo program of the last section are identical to steps 4 and 5. The program can be shortened somewhat by using the "saved sequence" instructions (see 3.3.11). A 1101 instruction (start saved sequence) would be placed between 3 and 4, and a 1102 instruction (end saved sequence) between 5 and 6. Then steps 7 and 8 can be replaced by a 1103 instruction (execute saved sequence).

Any sequence of instructions can be saved in this manner and repeated as many times as desired with 1103 instructions. For example, the saved sequence feature can be used to produce a complete series of views of a structure at (say) 15° intervals about an axis. Note that the instructions between the start and stop instructions are *both executed and saved* the first time through.

2.4 Drawing the Cubane Structure: An Example

The novel compound cubane[4] (C_4H_4) has been crystallized and the structure determined.[5] The carbon-carbon bonds lie along the edges of a cube within experimental error. The compound crystallizes with the trigonal symmetry of space group $R\bar{3}$. One carbon and one hydrogen are in special positions along the $\bar{3}$ axis, and the remaining carbon and hydrogen are in general positions. Anisotropic temperature factor coefficients were fitted to the carbon atoms during the least-squares refinement of the structure, and isotropic temperature factors were used for the hydrogen atoms.

The cell parameters are

$$a = b = c = 5.34 \text{ A} ,$$

$$\alpha = \beta = \gamma = 72.26^\circ .$$

The equivalent positions of space group[6] $R\bar{3}$ are x, y, z; z, x, y; y, z, x; $\bar{x}, \bar{y}, \bar{z}$; $\bar{z}, \bar{x}, \bar{y}$; and $\bar{y}, \bar{z}, \bar{x}$.

The positional parameters for C1, C2, H1, and H2 are given as −0.18711, 0.19519, 0.10706; 0.11546, 0.11546, 0.11546; −0.3246, 0.3468, 0.1848; and 0.2100, 0.2100, 0.2100, respectively. The anisotropic temperature factors given for the carbon atoms are of the type called zero[7] in this report (see 3.2.4.2). The coefficients b_{11}, b_{22}, b_{33}, b_{12}, b_{13}, b_{23} for C1 and C2 are 0.0410, 0.0425, 0.0450, −0.0042, −0.0142, −0.0051; and 0.0468, 0.0468, 0.0468, −0.0143, −0.0143, −0.0143.

2.4.1 Data Input for Cubane. – *2.4.1.1 Title Card* (see 3.2.1). – FORMAT (12A6)

Card No.

(1) CUBANE (E. B. FLEISCHER (1964) J. A. C. S. 86, 3889)

2.4.1.2 Cell Parameter Card (see 3.2.2). – FORMAT (6F9.6)

(2) 5.34 5.34 5.34 72.26 72.26 72.26

2.4.1.3 Symmetry Cards (see 3.3.3)

FORMAT (I1, F14.10, 3F3.0, 2(F15.10, 3F3.0))

(3) 0 0. 1 0 0 0. 0 1 0 0. 0 0 1

(4) 0 0. 0 0 1 0. 1 0 0 0. 0 1 0

---

[4] P. Eaton and T. Cole, *J. Am. Chem. Soc.* **86**, 3157 (1964).

[5] E. B. Fleischer, *J. Am. Chem. Soc.* **86**, 3889 (1964).

[6] N. F. M. Henry and K. Lonsdale (eds.), *International Tables for X-Ray Crystallography*, vol. I, Kynoch, Birmingham, 1962.

[7] Unfortunately, many authors of structure papers neglect to define the equation for the anisotropic temperature factor coefficients. In the present case, the type can be determined from the comparative isotropic temperature factor listed in anisotropic form in their Table I. In other instances one must arbitrarily choose a type (usually 0, 1, or 4 in the U.S.A.) and do the principal axis transformation, then check that the principal values are correct, or at least reasonable. In particular, the principal values must all be positive.

Card No.				
(5)	0	0. 0 1 0	0. 0 0 1	0. 1 0 0
(6)	0	0. −1 0 0	0. 0 −1 0	0. 0 0 −1
(7)	0	0. 0 0 −1	0. −1 0 0	0. 0 −1 0
(8)	1	0. 0 −1 0	0. 0 0 −1	0. −1 0 0

2.4.1.4 Atomic Parameter Cards. –

Positional parameters (see 3.3.4.1): FORMAT (A6, 3X,5F9.6,F9.0)

Thermal parameters (see 3.2.4.2): FORMAT (I1, F8.6,5F9.6,F9.0)

Atoms 1 and 2 are entered with positional parameters type 0 and anisotropic temperature factors type 0.

Card No.								
(9)		C1				−.18711	.19519	.10706	0
(10)	0		.04100	.04250	.04500	−.00420	−.01420	−.00510	0
(11)		C2				.11546	.11546	.11546	0
(12)	0		.04680	.04680	.04680	−.01430	−.01430	−.01430	0

Atoms 3 and 4 are entered with positional parameters type 0 and with dummy sphere temperature factors (type 7) 0.1 A in radius.

(13)		H1				−.32460	.34680	.18480	0
(14)	0		.1						7
(15)		H2				.21000	.21000	.21000	0
(16)	0		.1						7

Atom 5 is a dummy atom at the cell origin with a blank card dummy sphere (see last paragraph of 3.2.4.2). This could also be entered with type 7 as were atoms 3 and 4.

(17)		ORGN				.00000	.00000	.00000	0
(18)	1								0

In the card deck for this sample program, extensive use of Format No. 3 trailer cards (see 3.3.1) is made as a method of including a comment with an instruction. This convention is not mandatory, but it is a convenient method for annotating a program. This example uses a wide range of instructions in order to demonstrate them. As in the case with any programming system, there are many ways of doing any given problem. The Formats are described in 3.3.

2.4.2 Analysis of Structure (see 3.3.2). – These instructions are not connected with producing the figure. They are shown here just to demonstrate how they are used. A 101 instruction is used to obtain a tabulation of the atoms surrounding one atom or a series of several designated atoms. To obtain a list of all atoms (hydrogen and carbon atoms) out to a limit of (say) 3.61 A about the two carbons C1 and C2, one would use the following instruction. (The notation is explained in Section 3.3.2.)

Card No.

(19) 101 155501 2 1 4 3.61

Atoms 1 through 2 of symmetry operation 1 — Atoms 1 through 4 of all symmetry and translation operations — *D* max

A 102 instruction gives both interatomic distances and interatomic angles. In order to find all covalent bonds and bond angles about the two carbons we might use the following instruction.

(20) 102 155501 2 1 4 1.8

In this case a smaller *D* max was used so that only the distances and angles of immediate interest would be computed.

2.4.3 Programming the Cubane Illustration. – First we must initialize the plotter package.

(21) 201

The two plot boundary dimensions can be equal for the present illustration since the cubane molecule is a cube. Suppose we use an 11- by 11-in. boundary and specify a 1-in. margin to give a total working area of 9 by 9 in. A 24-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 24 1

In general we would use retracing to make the lettering, and certain other details, stand out more prominently. However, for the test example we will eliminate the retracing so that the illustration will plot as fast as possible.

(23) 303 0

The subject of the illustration is a single cubane molecule, which we will now define. One way of designating this subject is to specify a sphere of enclosure, centered on the dummy atom 555501, which is at the center of a cubane molecule. A radius of 3.2 A should be adequate to isolate a single molecule.

Card No.

(24) 402 555501 5 1 4 3.2

(a) (b) (c)

where the several parts designate:

(a) a run of origin atom (center of sphere) from atom 5 to atom 5 in symmetry position 55501 (that is, in this example, a single sphere),

(b) a run of target atom from atom 1 to atom 4, and

(c) a sphere radius of 3.2 A.

To orient the molecule, we will first define a coordinate system along the edges of the cubane cube. We will then rotate the molecule relative to this coordinate system to minimize overlap.

The origin of the coordinate system will be positioned on the dummy atom No. 5. The desired coordinate system orientation will be defined by specifying two vectors from the special position atom 255501 to the two symmetry-related general-position atoms 155501 and 155502.

(25) 501 555501 255501 155501 255501 155502 0 0

A rotation of 25° about the Y axis (axis 2) followed by a rotation of 28° about the X axis (axis 1) will produce a satisfactory view of the molecule.

(26) 502 2 25 1 28

The stereoscopic rotation for the left eye can be done at this point just to keep the instructions in numerical order. We will use a rotation of 3° about the Y axis (axis 2) for the left-eye view. Later in the program, we will make a $-3°$ rotation about the same axis for the right-eye view to give a total interocular angle of 6°.

(27) 503 2 3.0

To scale and position the subject for projection onto the drawing board, we will use two instructions. The first will automatically scale and position the subject to utilize all available space. The second will shrink the scale slightly to allow more space along the border.

A 604 instruction will automatically set X0, Y0, and SCAL1. However, the ellipsoid scale factor ratio SCAL2 must be specified independently. If we want thermal ellipsoids corresponding to 50% probability, then we will enter 1.54 for SCAL2.

(28) 604 0 0 0 1.54

To shrink the overall scale factor (SCAL1) by 10% we use the incremental instruction 611 and enter 0.9 for SCAL1.

Card No.

(29) 611 0 0 .9 0

This completes the composition of the illustration.

Since the structure will be drawn twice, once for each eye, the "saved sequence" feature can be used to shorten the program. Note that the instructions between the start and stop instructions are both *executed and saved* the first time through. They can then be re-executed as many times as desired by using the "execute saved sequence" instruction 1103.

The 1101 instruction starts the saved sequence.

(30) 1101

The ATOMS list currently contains all the atom designators for one cubane molecule. We want to draw the molecule in two separate steps so that the hydrogen and carbon atoms can be given different graphical representations. To eliminate the hydrogens from the list we use a sphere-of-enclosure elimination instruction and include only the hydrogens in its target list. This will leave only the carbon atom designators in the atoms list.

(31) 412 555501 5 3 4 3.2

To draw the carbon atoms we will construct a special code that (*a*) draws the three principal-plane forward traces and the boundary-plane trace (NPLANE = 4), (*b*) omits the reverse sides of the principal planes (NDOT = 0), (*c*) draws the forward principal axes without additional shading (NLINE = 1), and (*d*) omits the reverse principal axes (NDASH = 0). In addition we want the chemical symbols to be drawn with letters 0.2 in. high (before projection) and displaced from the atomic center by 0.6 in. in the horizontal direction and 0.7 in. in the vertical direction.

(32) 715 4 0 1 0 .2 .6 .7

The 715 instruction is used, rather than 705, to shorten the output listing of the example. Normally we would use the 705 to obtain a listing of all coordinates.

To draw the hydrogen atoms we must first clear the atoms array.

(33) 410

We then rebuild it with hydrogen atom designators alone. We could use a sphere of enclosure; however, for variety we will use an atom designator code run instead. The atom numbers run from 3 through 4 and the symmetry operators run from 1 through 6. All atoms will be in cell 555; consequently, there are no translation runs. Since one of the atoms (atom 4) is in a special position, duplicate entries will occur; but they are eliminated automatically.

Card No.

(34) 401 355501 – 455506

Since the hydrogen atoms are to be drawn with a standard model, the construction details will be taken care of automatically. We want chemical symbols 0.2 in. high and offset 0.35 in. horizontally and 0.4 in. vertically.

(35) 712 0 0 0 0 .2 .35 .4

Before drawing the bonds, we must reconstruct the complete molecule. This can be accomplished with a sphere of enclosure identical to the original one. The hydrogens that are already in the atoms list will not cause complications, since duplicates are automatically eliminated.

(36) 402 555501 5 1 4 3.2

The most convenient procedure for drawing bonds is to use the implicit bond instruction 812. All other information can be entered with a single format No. 2 trailer card (vector search code card).

(37) 2 812

(38) 0 $\underbrace{1 \quad 4}_{(a)}$ $\underbrace{1 \quad 4}_{(b)}$ $\underbrace{4}_{(c)}$ $\underbrace{.9 \quad 1.6}_{(d)}$ $\underbrace{.04}_{(e)}$

where

(*a*) and (*b*) are atom number runs for atom-pair bonds to be drawn,

(*c*) denotes bond type 4,

(*d*) denotes the distance range 0.9 to 1.6 A, which will cover all covalent bond distances, and

(*e*) the bond radius, is 0.04 A.

The remaining fields in the card can be blank, since a complete set of bond distance labels is not desired.

Because of the symmetry, there are only two different C – C bond lengths in cubane. These are C1-C1 and C1-C2. We shall label one example of each of these bonds. For variety let us label one with a normal bond-length label and the other with a perspective label. The two bonds which can be labeled most advantageously are (*a*) 155504 → 155503 and (*b*) 255504 → 155505. The labels will be 0.15 in. in height and displaced vertically from the bond center by – 0.4 in.

(39) 906 155504 155503 0 0 .15 0 –.4

(40) 916 255504 155505 0 0 .15 0 –.4

The final feature to be drawn is a caption (CUBANE) for the illustration. This can conveniently be positioned by "hanging" it from the dummy atom 555501 and "bouncing" it 1 in. off the lower y boundary.

Card No.									
(41)	3	902	555501	0	0	1.	.25	0	0
(42)				CUBANE					

The saved sequence can now be terminated.

(43) 1102

The plotter is then advanced 9 in. along x in preparation for the right-eye view.

(44) 202 9

The stereo rotation of $-3°$ about axis 2 is now performed in preparation for the right-eye view. (Note that this rotation starts with the reference orientation, not the previous working orientation.)

(45) 503 2 −3.0

The saved sequence can now be repeated for the right eye. Note that the atom list now contains the same information that it did when the first view was drawn.

(46) 1103

The illustration is now complete. The plotter is next advanced 20 in. along x to remove this figure from the working area.

(47) 202 20

A dummy plot for the CalComp system is now added to aid in stopping the CalComp plotter.

(48) 202 0

Finally we terminate the job and exit from the program.

(49) −1

2.4.4 Stereoscopic Illustration of Cubane. – Figure 2.1 shows the stereoscopic pair exactly as it was plotted by the CalComp 580 system. Figure 2.2 shows the same illustration after it was "touched up" by hand to correct for overlap.

Note that one bond distance label was drawn in perspective along the bond, and the other was drawn as a regular label parallel to the page.

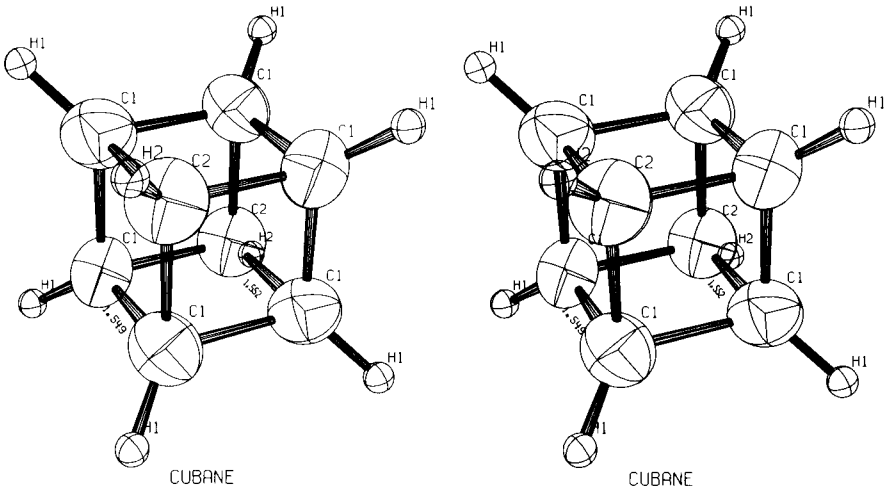

Fig. 2.1. The Sample Figure Cubane Before Retouching.

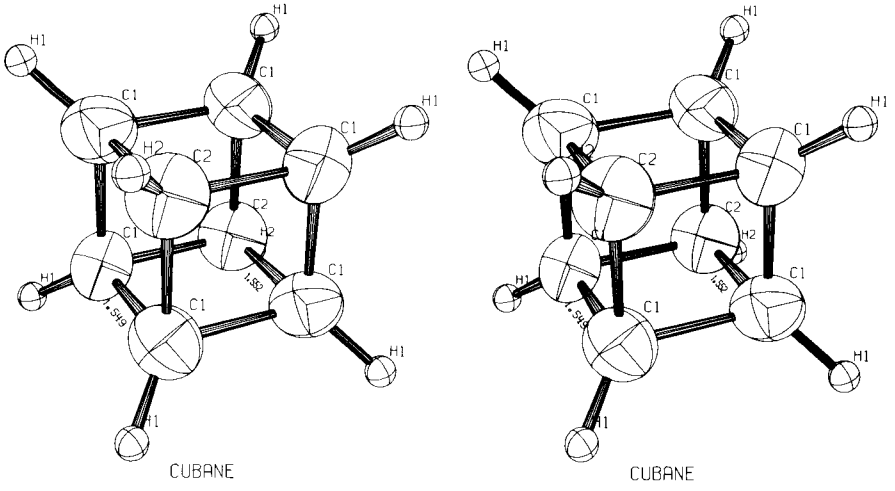

Fig. 2.2. The Sample Figure Cubane After Retouching.

2.4.5 Listing of Sample Input and Output. – *2.4.5.1 Listing of Input Cards.* –

```
  CUBANE (E.B.FLEISCHER  (1964) J.A.C.S  86,3889)                          EXAM0010
     5.34      5.34      5.34     72.26     72.26     72.26                 EXAM0020
               0  1  0  0                0  0  1  0                0  0  0  1EXAM0030
               0  0  0  1                0  1  0  0                0  0  1  0EXAM0040
               0  0  1  0                0  0  0  1                0  1  0  0EXAM0050
               0 -1  0  0                0  0 -1  0                0  0  0 -1EXAM0060
               0  0  0 -1                0 -1  0  0                0  0 -1  0EXAM0070
1              0  0 -1  0                0  0  0 -1                0 -1  0  0EXAM0080
  C1                            -.18711   .19519   .10706         0         EXAM0090
   .04100    .04250    .04500  -.00420  -.01420  -.00510         0         EXAM0100
  C2                             .11546   .11546   .11546         0         EXAM0110
   .04680    .04680    .04680  -.01430  -.01430  -.01430         0         EXAM0120
  H1                            -.32460   .34680   .18480         0         EXAM0130
      .10                                                          7         EXAM0140
  H2                             .21000   .21000   .21000         0         EXAM0150
      .10                                                          7         EXAM0160
 ORGN                                 0        0        0         0         EXAM0170
1                                                                 0         EXAM0180
  3   101   155501        2        1        4      3.61                    EXAM0190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****         EXAM0200
  3   102   155501        2        1        4      1.8                     EXAM0210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****             EXAM0220
  3   201                                                                 EXAM0230
***** INITIALIZE CALCOMP PLOT PACKAGE *****                                EXAM0240
  3   301      11.      11.      24.       1.                             EXAM0250
***** 11X11 BOUNDARY, 9X9 INSIDE 1 INCH MARGIN, VIEW FROM 24 INCHES ****EXAM0260
  3   303        0                                                        EXAM0270
***** ELIMINATE ALL RETRACING *****                                        EXAM0280
  3   402   555501        5        1        4      3.2                     EXAM0290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5 *****             EXAM0300
  3   501   555501   255501   155501   255501   155502                   0EXAM0310
***** ORGN AT DUMMY ATOM 5, VECTORS ALONG 2 EDGES OF CUBANE *****          EXAM0320
  3   502        2      25.        1      28.                             EXAM0330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT X *****             EXAM0340
  3   503        2      3.0                                               EXAM0350
***** STEREO ROTATION OF 3.0 DEGREES ABOUT Y FOR LEFT EYE *****            EXAM0360
  3   604        0        0        0     1.54                             EXAM0370
***** AUTO SCALE AND POSITION TO 9X9. 50 PERCENT PROBABILITY ELLIPSOIDS EXAM0380
  3   611        0        0       .9        0                             EXAM0390
***** SHRINK SCALE BY 10 PERCENT FOR SAFETY *****                          EXAM0400
  3  1101                                                                 EXAM0410
***** START SAVE SEQUENCE *****                                            EXAM0420
  3   412   555501        5        3        4      3.2                     EXAM0430
***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION *****           EXAM0440
  3   715        4        0        1        0      .20      .60      .70EXAM0450
***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. *****    EXAM0460
  3   410                                                                 EXAM0470
***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECEMEAL *****     EXAM0480
  3   401   355501  -455506                                               EXAM0490
***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN *****             EXAM0500
  3   712                                                 .2      .35      .40EXAM0510
***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH *****     EXAM0520
  3   402   555501        5        1        4      3.2                     EXAM0530
***** ENCLOSER SPHERE WITH COMPLETE MODEL *****                            EXAM0540
  2   812                                                                 EXAM0550
  3        1  4  1  4  4     .9   1.6   .04                               EXAM0560
***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG ***** EXAM0570
  3   906   155504   155503        0        0      .15        0      -.4EXAM0580
***** LABEL UNIQUE C-C BONDS .   CAPTION # CUBANE *****                    EXAM0590
      916   255504   155505        0        0      .15        0      -.4EXAM0600
  3   902   555501        0        0      1.0      .25        0        0EXAM0610
                                CUBANE                                    EXAM0620
  3  1102                                                                 EXAM0630
***** END OF SAVE SEQUENCE *****                                          EXAM0640
  3   202       9.                                                        EXAM0650
```

```
***** ADVANCE PLOTTER 9 INCHES ALONG X FOR RIGHT EYE VIEW *****          EXAM0660
  3   503        2     -3.0                                             EXAM0670
***** STEREO ROTATICN FOR RIGHT EYE *****                               EXAM0680
  3  1103                                                               EXAM0690
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE VIEW *****                   EXAM0700
  3   202      20.                                                      EXAM0710
***** ADVANCE PLOTTER 20 INCHES *****                                   EXAM0720
  3   202        0                                                      EXAM0730
***** ADDS DUMMY PLOT TO MAGNETIC TAPE *****                            EXAM0740
       -1                                                               EXAM0750
```

2.4.5.2 Listing of Output from the Monitor Output Tape of the Computer. –

```
CUBANE (E.B.FLEISCHER  (1964) J.A.C.S  86,3889)

DIRECT CELL PARAMETERS
     A              B              C              ALPHA          BETA           GAMMA
 5.340000       5.340000       5.340000         72.260         72.260         72.260
                                          COSINE  0.30469811     0.30469811     0.30469811

RECIPROCAL CELL PARAMETERS
     A*             B*             C*             ALPHA*         BETA*          GAMMA*
 0.202207       0.202207       0.202207        103.506        103.506        103.506
                                          COSINE -0.23353916    -0.23353916    -0.23353916

SYMMETRY TRANSFORMATIONS
    NO.            TRANSFORMED X                    TRANSFORMED Y                    TRANSFORMED Z
     1     0.        1. X  0. Y  0. Z     0.        0. X  1. Y  0. Z     0.        0. X  0. Y  1. Z
     2     0.        0. X  0. Y  1. Z     0.        1. X  0. Y  0. Z     0.        0. X  1. Y  0. Z
     3     0.        0. X  1. Y  0. Z     0.        0. X  0. Y  1. Z     0.        1. X  0. Y  0. Z
     4     0.       -1. X  0. Y  0. Z     0.        0. X -1. Y  0. Z     0.        0. X  0. Y -1. Z
     5     0.        0. X  0. Y -1. Z     0.       -1. X  0. Y  0. Z     0.        0. X -1. Y  0. Z
     6     0.        0. X -1. Y  0. Z     0.        0. X  0. Y -1. Z     0.       -1. X  0. Y  0. Z

NO. ATOM        X          Y          Z          B11        B22        B33        B12        B13        B23   TYPE
 1   C1    -0.187110   0.195190   0.107060   0.041000   0.042500   0.045000  -0.004200  -0.014200  -0.005100   0.
 2   C2     0.115460   0.115460   0.115460   0.046800   0.046800   0.046800  -0.014300  -0.014300  -0.014300   0.
 3   H1    -0.324600   0.346800   0.184800   0.100000  -0.         -0.        -0.        -0.        -0.         7.
 4   H2     0.210000   0.210000   0.210000   0.100000  -0.         -0.        -0.        -0.        -0.         7.
 5  ORGN    0.         0.         0.        -0.        -0.         -0.        -0.        -0.        -0.         0.

NO. ATOM        X          Y          Z          RMSD 1     RMSD 2     RMSD 3
 1   C1    -0.187110   0.195190   0.107060   0.204899   0.239856   0.255794
 2   C2     0.115460   0.115460   0.115460   0.205704   0.247733   0.247733
 3   H1    -0.324600   0.346800   0.184800   0.100000   0.100000   0.100000
 4   H2     0.210000   0.210000   0.210000   0.100000   0.100000   0.100000
 5  ORGN    0.         0.         0.         0.100000   0.100000   0.100000

CUBANE (E.B.FLEISCHER  (1964) J.A.C.S  86,3889)

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR          Y VECTOR          Z VECTOR
   0.1872659E-00  -0.5990827E-01  -0.4722319E-01          0.5340000E 01   0.4470348E-07   0.2980232E-07
   0.               0.1966152E-00  -0.4722319E-01          0.1627088E 01   0.5086078E 01   0.2980232E-07
   0.               0.               0.2022067E-00          0.1627088E 01   0.1187798E 01   0.4945434E 01

(((((  INSTRUCTION  101  )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.3610000E 01 -0.          -0.

***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****

     FROM ATOMS     TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE (MIN  MAX)    (MIN  MAX)                          A         B         C
```

```
101  155501    2      1    4                        3.610   -0.      -0.

VECTORS FROM ATOM  (  1,55501)      TO ATOMS   1 THROUGH   4
     C1      H1     (  1,55501)-0.1871 0.1952 0.1071     (  3,55501)-0.3246 0.3468 0.1848       D # 1.012
     C1      C1                                          (  1,55505)-0.1071 0.1871-0.1952       D # 1.549
     C1      C1                                          (  1,55506)-0.1952-0.1071 0.1871       D # 1.549
     C1      C2                                          (  2,55501) 0.1155 0.1155 0.1155       D # 1.552
     C1      C1                                          (  1,55502) 0.1071-0.1871 0.1952       D # 2.183
     C1      C1                                          (  1,55503) 0.1952 0.1071-0.1871       D # 2.183
     C1      C2                                          (  2,55504)-0.1155-0.1155-0.1155       D # 2.202
     C1      H1                                          (  3,55506)-0.3468-0.1848 0.3246       D # 2.282
     C1      H1                                          (  3,55505)-0.1848 0.3246-0.3468       D # 2.306
     C1      H2                                          (  4,55501) 0.2100 0.2100 0.2100       D # 2.376
     C1      C1                                          (  1,55504) 0.1871-0.1952-0.1071       D # 2.677
     C1      H1                                          (  3,55502) 0.1848-0.3246 0.3468       D # 3.052
     C1      H1                                          (  3,55503) 0.3468 0.1848-0.3246       D # 3.069
     C1      H2                                          (  4,45501)-0.7900 0.2100 0.2100       D # 3.077
     C1      H2                                          (  4,56504)-0.2100 0.7900-0.2100       D # 3.096
     C1      H2                                          (  4,55504)-0.2100-0.2100-0.2100       D # 3.175
     C1      H1                                          (  3,55605)-0.1848 0.3246 0.6532       D # 3.200
     C1      H1                                          (  3,45603)-0.6532 0.1848 0.6754       D # 3.284
     C1      H1                                          (  3,46504)-0.6754 0.6532-0.1848       D # 3.388
     C1      C2                                          (  2,56504)-0.1155 0.8845-0.1155       D # 3.609

VECTORS FROM ATOM  (  2,55501)      TO ATOMS   1 THROUGH   4
     C2      H2     (  2,55501) 0.1155 0.1155 0.1155     (  4,55501) 0.2100 0.2100 0.2100       D # 1.109
     C2      C1                                          (  1,55501)-0.1871 0.1952 0.1071       D # 1.552
     C2      C1                                          (  1,55502) 0.1071-0.1871 0.1952       D # 1.552
     C2      C1                                          (  1,55503) 0.1952 0.1071-0.1871       D # 1.552
     C2      C1                                          (  1,55504) 0.1871-0.1952-0.1071       D # 2.202
     C2      C1                                          (  1,55505)-0.1071 0.1871-0.1952       D # 2.202
     C2      C1                                          (  1,55506)-0.1952-0.1071 0.1871       D # 2.202
     C2      H1                                          (  3,55501)-0.3246 0.3468 0.1848       D # 2.273
     C2      H1                                          (  3,55502) 0.1848-0.3246 0.3468       D # 2.273
     C2      H1                                          (  3,55503) 0.3468 0.1848-0.3246       D # 2.273
     C2      C2                                          (  2,55504)-0.1155-0.1155-0.1155       D # 2.710
     C2      H1                                          (  3,55504) 0.3246-0.3468-0.1848       D # 3.091
     C2      H1                                          (  3,55505)-0.1848 0.3246-0.3468       D # 3.091
     C2      H1                                          (  3,55506)-0.3468-0.1848 0.3246       D # 3.091
     C2      H1                                          (  3,56504) 0.3246 0.6532-0.1848       D # 3.181
     C2      H1                                          (  3,55605)-0.1848 0.3246 0.6532       D # 3.181
     C2      H1                                          (  3,65506) 0.6532-0.1848 0.3246       D # 3.181
     C2      C1                                          (  1,56504) 0.1871 0.8048-0.1071       D # 3.609
     C2      C1                                          (  1,55605)-0.1071 0.1871 0.8048       D # 3.609
     C2      C1                                          (  1,65506) 0.8048-0.1071 0.1871       D # 3.609

((((( INSTRUCTION  102 )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.1800000E 01 -0.          -0.

***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****

     FROM ATOMS    TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE (MIN  MAX)   (MIN  MAX)                          A        B        C
```

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```
102  155501    2      1    4                          1.800   -0.      -0.

VECTORS FROM ATOM  (  1,55501)      TO ATOMS   1 THROUGH   4
     C1      H1     (  1,55501)-0.1871 0.1952 0.1071      (  3,55501)-0.3246 0.3468 0.1848        D # 1.012
     C1      C1                                           (  1,55505)-0.1071 0.1871-0.1952        D # 1.549
     C1      C1                                           (  1,55506)-0.1952-0.1071 0.1871        D # 1.549
     C1      C2                                           (  2,55501) 0.1155 0.1155 0.1155        D # 1.552

ANGLES AROUND ATOM     1
     H1      C1      C1            (  3,55501) (  1,55501) (  1,55505)                                124.69
     H1      C1      C1            (  3,55501) (  1,55501) (  1,55506)                                127.16
     H1      C1      C2            (  3,55501) (  1,55501) (  2,55501)                                123.52
     C1      C1      C1            (  1,55505) (  1,55501) (  1,55506)                                 89.60
     C1      C1      C2            (  1,55505) (  1,55501) (  2,55501)                                 90.48
     C1      C1      C2            (  1,55506) (  1,55501) (  2,55501)                                 90.48

VECTORS FROM ATOM  (  2,55501)      TO ATOMS   1 THROUGH   4
     C2      H2     (  2,55501) 0.1155 0.1155 0.1155      (  4,55501) 0.2100 0.2100 0.2100        D # 1.109
     C2      C1                                           (  1,55501)-0.1871 0.1952 0.1071        D # 1.552
     C2      C1                                           (  1,55502) 0.1071-0.1871 0.1952        D # 1.552
     C2      C1                                           (  1,55503) 0.1952 0.1071-0.1871        D # 1.552

ANGLES AROUND ATOM     2
     H2      C2      C1            (  4,55501) (  2,55501) (  1,55501)                                125.66
     H2      C2      C1            (  4,55501) (  2,55501) (  1,55502)                                125.66
     H2      C2      C1            (  4,55501) (  2,55501) (  1,55503)                                125.66
     C1      C2      C1            (  1,55501) (  2,55501) (  1,55502)                                 89.44
     C1      C2      C1            (  1,55501) (  2,55501) (  1,55503)                                 89.44
     C1      C2      C1            (  1,55502) (  2,55501) (  1,55503)                                 89.44

((((( INSTRUCTION  201 )))))
     -0.          -0.          -0.          -0.          -0.          -0.          -0.

     ***** INITIALIZE CALCOMP PLOT PACKAGE *****

((((( INSTRUCTION  301 )))))
      0.1100000E 02  0.1100000E 02  0.2400000E 02  0.1000000E 01 -0.          -0.          -0.

     ***** 11X11 BOUNDARY, 9X9 INSIDE 1 INCH MARGIN, VIEW FROM 24 INCHES ****

     PLOT LIMITS 11.00 BY 11.00 IN.  INCLUDING  1.00  IN. MARGIN
     VIEW DISTANCE 24.000 INCHES

((((( INSTRUCTION  303 )))))
      0.          -0.          -0.          -0.          -0.          -0.          -0.

     ***** ELIMINATE ALL RETRACING *****

     RETRACE DISPLACEMENT # 0.     INCH
```

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```
((((( INSTRUCTION  402 )))))
 0.5555010E 06  0.5000000E 01  0.1000000E 01  0.4000000E 01  0.3200000E 01 -0.            -0.

***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5 *****

     FROM ATOMS    TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE (MIN  MAX)   (MIN  MAX)                          A        B        C

402  555501    5      1    4                       3.200   -0.      -0.

VECTORS FROM ATOM  (  5,55501)      TO ATOMS   1 THROUGH   4

CONTENTS OF ATOMS ARRAY
       155501.   255501.   355501.   455501.   155502.   355502.   155503.   355503.   155504.   255504.
       355504.   455504.   155505.   355505.   155506.   355506.

((((( INSTRUCTION  501 )))))
 0.5555010E 06  0.2555010E 06  0.1555010E 06  0.2555010E 06  0.1555020E 06 -0.            0.

***** ORGN AT DUMMY ATOM 5, VECTORS ALONG 2 EDGES OF CUBANE *****

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR          Y VECTOR          Z VECTOR
  -0.1950172E-00  -0.5332417E-01   0.3517815E-02          -0.5161574E 01   0.2128974E-00   0.1352193E 01
   0.5138884E-01   0.4031208E-02   0.1955262E-00          -0.2760937E-00   0.1350080E 01   0.5159133E 01
  -0.5414101E-02   0.1954783E-00  -0.5144393E-01          -0.1402323E 01   0.5145891E 01   0.2624691E-00

((((( INSTRUCTION  502 )))))
 0.2000000E 01  0.2500000E 02  0.1000000E 01  0.2800000E 02 -0.            -0.            -0.

***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT X *****

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR          Y VECTOR          Z VECTOR
  -0.1752589E-00  -0.8727205E-01   0.5055148E-01          -0.4106513E 01  -0.1411455E 01   0.3108044E 01
   0.1292070E-00  -0.6943834E-01   0.1391812E-00           0.1930118E 01  -0.1057867E 01   0.4865301E 01
  -0.2664798E-01   0.1934115E-00   0.5262520E-01          -0.1160012E 01   0.4153645E 01   0.3149160E 01

((((( INSTRUCTION  503 )))))
 0.2000000E 01  0.3000000E 01 -0.            -0.            -0.            -0.            -0.

***** STEREO ROTATION OF 3.0 DEGREES ABOUT Y FOR LEFT EYE *****

ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                  POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR          Y VECTOR          Z VECTOR
  -0.1723731E-00  -0.8727205E-01   0.5965454E-01          -0.3938223E 01  -0.1411455E 01   0.3318703E 01
   0.1363141E-00  -0.6943834E-01   0.1322283E-00           0.2182103E 01  -0.1057867E 01   0.4757619E 01
  -0.2385727E-01   0.1934115E-00   0.5394772E-01          -0.9936078E 00   0.4153645E 01   0.3205554E 01

((((( INSTRUCTION  604 )))))
 0.            0.            0.            0.1540000E 01 -0.            -0.            -0.
```

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```
***** AUTO SCALE AND POSITION TO 9X9. 50 PERCENT PROBABILITY ELLIPSOIDS

ORIGIN POINT IN PLOTTER COORD.(  5.26 ,  5.89 ) IN.
OVERALL SCALE # 2.196 INCH/ANGSTROM ELLIPSOID SCALE # 1.540
VIEW DISTANCE 24.000 INCHES

((((( INSTRUCTION  611 )))))
 0.            0.            0.9000000E 00  0.            -0.            -0.            -0.

***** SHRINK SCALE BY 10 PERCENT FOR SAFETY *****

ORIGIN POINT IN PLOTTER COORD.(  5.26 ,  5.89 ) IN.
OVERALL SCALE # 1.977 INCH/ANGSTROM ELLIPSOID SCALE # 1.540
VIEW DISTANCE 24.000 INCHES

((((( INSTRUCTION 1101 )))))
-0.           -0.           -0.           -0.           -0.           -0.           -0.

***** START SAVE SEQUENCE *****

((((( INSTRUCTION  412 )))))
 0.5555010E 06  0.5000000E 01  0.3000000E 01  0.4000000E 01  0.3200000E 01 -0.           -0.

***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION *****

     FROM ATOMS    TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE (MIN  MAX)   (MIN  MAX)                          A        B        C

412  555501    5      3    4                      3.200   -0.      -0.


VECTORS FROM ATOM  (  5,55501)      TO ATOMS   3 THROUGH   4

CONTENTS OF ATOMS ARRAY
       155501.   255501.   155502.   155503.   155504.   255504.   155505.   155506.

((((( INSTRUCTION  715 )))))
 0.4000000E 01  0.            0.1000000E 01  0.            0.2000000E-00  0.6000000E 00  0.7000000E 00

***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. *****

((((( INSTRUCTION  410 )))))
-0.           -0.           -0.           -0.           -0.           -0.           -0.

***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECEMEAL *****

((((( INSTRUCTION  401 )))))
 0.3555010E 06 -0.4555060E 06 -0.           -0.           -0.           -0.           -0.

***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN *****

CONTENTS OF ATOMS ARRAY
       355501.   455501.   355502.   355503.   355504.   455504.   355505.   355506.
```

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```
((((( INSTRUCTION  712 )))))
     -0.            -0.            -0.            -0.            0.2000000E-00  0.3500000E-00  0.4000000E-00

     ***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH *****

((((( INSTRUCTION  402 )))))
      0.5555010E 06  0.5000000E 01  0.1000000E 01  0.4000000E 01  0.3200000E 01 -0.            -0.

     ***** ENCLOSER SPHERE WITH COMPLETE MODEL *****

          FROM ATOMS    TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
     CODE (MIN  MAX)   (MIN  MAX)                          A        B        C

     402  555501    5      1    4                      3.200   -0.      -0.

     VECTORS FROM ATOM  (  5,55501)      TO ATOMS   1 THROUGH   4

     CONTENTS OF ATOMS ARRAY
            355501.   455501.   355502.   355503.   355504.   455504.   355505.   355506.   155501.   255501.
            155502.   155503.   155504.   255504.   155505.   155506.

((((( INSTRUCTION  812 )))))
     -0.            -0.            -0.            -0.            -0.            -0.            -0.
        1  4  1  4  4    0.90000    1.60000    0.04000   -0.        -0.        -0.        -0.        -0.

     ***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG *****

     BOND SELECTION CODES

     (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
     (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
          1    4       1    4       4  0.90  1.60   0.040  -0.     -0.     -0.     -0.       -0.
     FAULT NG # 14   455504.   800


((((( INSTRUCTION  906 )))))
      0.1555040E 06  0.1555030E 06  0.            0.            0.1500000E-00  0.            -0.4000000E-00

     ***** LABEL UNIQUE C-C BONDS .   CAPTION # CUBANE *****

((((( INSTRUCTION  916 )))))
      0.2555040E 06  0.1555050E 06  0.            0.            0.1500000E-00  0.            -0.4000000E-00

((((( INSTRUCTION  902 )))))
      0.5555010E 06  0.            0.            0.1000000E 01  0.2500000E-00  0.             0.

                                     CUBANE

((((( INSTRUCTION 1102 )))))
     -0.            -0.            -0.            -0.            -0.            -0.            -0.

     ***** END OF SAVE SEQUENCE *****
```

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```
((((( INSTRUCTION  202 )))))
      0.9000000E 01 -0.            -0.            -0.            -0.            -0.            -0.

     ***** ADVANCE PLOTTER 9 INCHES ALONG X FOR RIGHT EYE VIEW *****

((((( INSTRUCTION  503 )))))
      0.2000000E 01 -0.3000000E 01 -0.            -0.            -0.            -0.            -0.

     ***** STEREO ROTATION FOR RIGHT EYE *****

     ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                  POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1776644E-00  -0.8727205E-01   0.4130986E-01          -0.4263548E 01  -0.1411455E 01   0.2888866E 01
        0.1217458E-00  -0.6943834E-01   0.1457526E-00           0.1672843E 01  -0.1057867E 01   0.4959648E 01
       -0.2936565E-01   0.1934115E-00   0.5115843E-01          -0.1323236E 01   0.4153645E 01   0.3084133E 01

((((( INSTRUCTION 1103 )))))
     -0.            -0.            -0.            -0.            -0.            -0.            -0.

     ***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE VIEW *****

((((( INSTRUCTION  412 )))))
      0.5555010E 06  0.5000000E 01  0.3000000E 01  0.4000000E 01  0.3200000E 01 -0.            -0.

     ***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION *****

          FROM ATOMS    TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
     CODE (MIN  MAX)   (MIN  MAX)                          A        B        C

     412  555500    4      3    4                       3.200   -0.      -0.

     VECTORS FROM ATOM  (  5,55500)      TO ATOMS   3 THROUGH   4

     CONTENTS OF ATOMS ARRAY
            155501.   255501.   155502.   155503.   155504.   255504.   155505.   155506.

((((( INSTRUCTION  715 )))))
      0.4000000E 01  0.             0.9999999E 00  0.             0.2000000E-00  0.6000000E 00  0.7000000E 00

     ***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. *****

((((( INSTRUCTION  410 )))))
     -0.            -0.            -0.            -0.            -0.            -0.            -0.

     ***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECEMEAL *****

((((( INSTRUCTION  401 )))))
      0.3555010E 06 -0.4555060E 06 -0.            -0.            -0.            -0.            -0.

     ***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN *****
```

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```
CONTENTS OF ATOMS ARRAY
        355501.   455501.   355502.   355503.   355504.   455504.   355505.   355506.

((((( INSTRUCTION  712 )))))
-0.            -0.            -0.            -0.            0.2000000E-00  0.3500000E-00  0.4000000E-00

***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH *****

((((( INSTRUCTION  402 )))))
 0.5555010E 06  0.5000000E 01  0.9999999E 00  0.4000000E 01  0.3200000E 01 -0.            -0.

***** ENCLOSER SPHERE WITH COMPLETE MODEL *****

     FROM ATOMS    TO ATOMS       WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE (MIN  MAX)   (MIN  MAX)                          A        B        C

402  555500    4      1    4                      3.200   -0.      -0.


VECTORS FROM ATOM  (  5,55500)      TO ATOMS   1 THROUGH   4

CONTENTS OF ATOMS ARRAY
        355501.   455501.   355502.   355503.   355504.   455504.   355505.   355506.   155501.   255501.
        155502.   155503.   155504.   255504.   155505.   155506.

((((( INSTRUCTION  812 )))))
-0.            -0.            -0.            -0.            -0.            -0.            -0.
   1  4  1  4  4    0.90000    1.60000    0.04000   -0.        -0.        -0.        -0.        -0.

***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG *****

BOND SELECTION CODES

(SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
(  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
     1    4       1    4       4  0.90  1.60   0.040  -0.     -0.     -0.     -0.       -0.
FAULT NG # 14   455504.   800


((((( INSTRUCTION  906 )))))
 0.1555040E 06  0.1555030E 06  0.            0.            0.1500000E-00  0.            -0.4000000E-00

***** LABEL UNIQUE C-C BONDS .   CAPTION # CUBANE *****

((((( INSTRUCTION  916 )))))
 0.2555040E 06  0.1555050E 06  0.            0.            0.1500000E-00  0.            -0.4000000E-00

((((( INSTRUCTION  902 )))))
 0.5555010E 06  0.             0.            0.9999999E 00  0.2500000E-00  0.             0.

                                  CUBANE
```

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```
((((( INSTRUCTION 1102 )))))
      -0.            -0.            -0.            -0.            -0.            -0.            -0.

      ***** END OF SAVE SEQUENCE *****

((((( INSTRUCTION  202 )))))
       0.2000000E 02 -0.            -0.            -0.            -0.            -0.            -0.

      ***** ADVANCE PLOTTER 20 INCHES *****

((((( INSTRUCTION  202 )))))
       0.            -0.            -0.            -0.            -0.            -0.            -0.

      ***** ADDS DUMMY PLOT TO MAGNETIC TAPE *****

((((( INSTRUCTION   -1 )))))
```

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3. DETAILED OPERATING INSTRUCTIONS

3.1 Definitions

Several conventions must be defined before the instructions can be explained.

3.1.1 Atom Designator Code (ADC) and Addressable Point. – In order to specify a particular atom in the crystal within a reasonable distance from the crystallographically defined origin, the following five-component *a*tom *d*esignator code word (ADC) is used.

$$ADC = AN*10^5 + (TA + 5)*10^4 + (TB + 5)*10^3 + (TC + 5)*10^2 + SN$$

where

AN = *ATOM NUMBER* ($0 \leqq AN \leqq NATOM \leqq 200$) = the sequential number of the atom in the input list of atoms in the asymmetric unit, which contains NATOM atoms. Atom zero is not in the input atom list but refers to the crystal origin point (0., 0., 0.).

TA,TB,TC = *crystal lattice translation digits* along cell edges **a**, **b**, and **c**. Each digit in ADC can range from 1 to 9; consequently, it is possible to move up to ±4 lattice translations in any direction from the origin cell 5,5,5. In certain cases 0,0,0 is permitted in place of 5,5,5; however, a mixed translation designation such as 0,5,5 is not permitted.

SN = *symmetry operator number* ($0 \leqq SN \leqq NSYM \leqq 48$) = the numerical position of the symmetry operator in the input symmetry operator list which contains NSYM entries. Symmetry operator number zero is not in the input list but refers to an identity operator. However, the identity operation (corresponding to position *x, y, z*) must in general also be somewhere in the input symmetry operator list.

Example: An atom designation code of *3 475 02* refers to atom 3 moved through symmetry operation 2, then translated – 1 cell translation along **a**, +2 cell translations along **b**, and 0 cell translations along **c**.

An *addressable point* in the crystal is any point for which an atom designator code exists. In general, the addressable region is approximately a 9 × 9 × 9 block of unit cells.

3.1.2 Vector Designator Code (VDC). – A vector direction is specified by two atom designator codes. The vector direction is from the first to the second.

Example: 253704 263704 is a vector along the positive **a** direction of the crystal lattice.

3.1.3 Atom Designator Run (ADR). – A straight run sequence of atoms can be defined using two atom designator codes with a negative sign preceding the second of the two. The run hierarchy is: first, atom number AN; second, symmetry operation SN; third, **a** translation TA; fourth, **b** translation TB; and last, **c** translation TC.

Example: ADR (145502 – 245603) will generate the 8-atom run 145502, 245502, 145503, 245503, 145602, 245602, 145603, 245603.

3.1.4 Atom Number Run (ANR). – The Atom Number Run is a subset of the Atom Designator Run. In this case, only the atom number AN is allowed to change. Normally, an ANR is entered by using only the atom number (AN) values for the first and last members of the sequence without a minus sign.

Example: (1 4) will designate atoms 1, 2, 3, and 4 of the input list.

3.1.5 Vector Search Code (VSC). – A vector search code consists of two atom number runs and a distance range. It is used for finding interatomic distances which have a particular chemical significance, such as covalent and coordination bonds.

Example: Suppose that metal atoms are numbers 1 and 2 in the atom list and oxygen atoms are 6–12 and that the interatomic distance range between metals and oxygens is 1.9 A to 2.4 A. The metal-to-oxygen vectors can be specified by the vector search code (1 2) (6 12) (1.9 2.4). Several variations of this basic code are used in the program.

3.1.6 Sphere of Enclosure. – The sphere of enclosure specifies some or all of the atoms lying within a sphere of radius *D* max about a given "origin" atom without the necessity of delineating each atom individually. This "sphere of enclosure" is said to contain a *complete population* if all addressable atoms within the *D* max radius are included. If the sphere of enclosure contains only certain types of atoms which are derived from a group of sequential atoms in the input list, then the sphere is said to have a *partial population.* Finally, the population (complete or partial) of the sphere of enclosure can be screened as selectively as desired through the use of vector search codes (3.1.5), and the resulting content is called a *vector screened population.*

A sphere of enclosure can be centered on any addressable atom, but one should not use points in the outermost cells as centers because of the possibility of having nonaddressable points within the *D* max radius.

3.1.7 Box of Enclosure. – This is a rectangular parallelepiped which can be centered about any addressable point and assigned arbitrary orientation and dimensions. This "box of enclosure" can have a *complete population* or a *partial population* as described for the sphere of enclosure (3.1.6). However, vector screening is not allowed with the box of enclosure.

3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems. – Many of the OR TEP calculations use fractional coordinates based on the crystal axes **a**, **b**, and **c** (triclinic coordinate system); but other steps necessitate the introduction of orthonormal base vector triplets (Cartesian coordinate systems). Two Cartesian systems (reference and working) are utilized. The reference (major) system is used for all operations except plotting, where the working (minor) system is used. For a right-eye or left-eye stereo view, the working system is moved from the reference system by rotation about an axis of the reference system. However, certain decisions made while plotting must still be referred to the reference system to maintain accurate stereopsis. The user can define and orient the two Cartesian systems through the instructions of series 500. Until a 500-series instruction is given, a "standard Cartesian system" is utilized for both the reference and working systems. The orthonormal base vectors of the standard system are oriented as follows:

$$x \text{ axis along } \mathbf{a},$$
$$y \text{ axis along } (\mathbf{a} \times \mathbf{b}) \times \mathbf{a},$$
$$z \text{ axis along } (\mathbf{a} \times \mathbf{b}) = \mathbf{c}^*,$$

where **a**, **b**, and **c** are crystal axes and $\times$ denotes the outer vector product (cross product). The symbol $\mathbf{c}^*$ refers to a reciprocal axis.

3.1.9 Prime Parameters and Primer Constants. – In the process of mathematically describing an illustration to be machine drawn, many parameters must be used. The more basic among these parameters are called *Prime Parameters*. The values assigned to these prime parameters are often similar or identical from one problem to the next. The first thing OR TEP does is to call subroutine PRIME, which sets as many prime parameters as possible to reasonable, "in the ball park," *Primer Constants*. For example, the maximum plot dimensions (instruction 300 series) are set at 30.0 in. for x maximum and 11.0 in. for y maximum, and the overall scale for plotting (instruction 600 series) is set at 1.0 in./A. If the value assigned to a particular constant by the primer routine is satisfactory, the user does not have to reset this constant with OR TEP instructions.

3.2 Crystal Structure Data Input

3.2.1 Title Card. – FORMAT (12A6)

Columns	
1–72	Title consisting of any desired alphanumeric identification information. This will appear periodically in the output.

3.2.2 Cell Parameter Card. – FORMAT (6F9.6). Any one of the four following input alternatives may be used (no indicator is needed to specify which type).[1]

Columns	Type A	Type B	Type C	Type D
1–9	**a** (A)	**a** (A)	**a*** (A^{-1})	**a*** (A^{-1})
10–18	**b** (A)	**b** (A)	**b*** (A^{-1})	**b*** (A^{-1})
19–27	**c** (A)	**c** (A)	**c*** (A^{-1})	**c*** (A^{-1})
28–36	α (deg)	cos α	α^* (deg)	cos α^*
37–45	β (deg)	cos β	β^* (deg)	cos β^*
46–54	γ (deg)	cos γ	γ^* (deg)	cos γ^*

The parameters **a***, etc., refer to the reciprocal unit cell such that **a**·**a*** = 1. All four types will be printed out regardless of which type was used for input.

3.2.3 Symmetry Cards (1 ≦ NSYM ≦ 48). – FORMAT (I1,F14.10, 3F3.0,2(F15.10,3F3.0)). The card will be interpreted in one of two ways, depending on the numerical value of the number in columns 70–72. If that number is <5.0, the card is interpreted as a crystallographic symmetry operation; but if the number is ≧5.0, the card is interpreted as a general helix-screw symmetry operation[2] along the **c*** crystal axis[3]

[1]The routine assumes that **a** ≧ 1.0 A, **a*** < 1.0 A^{-1}, α (or α^*) ≧ 1.0°, and $|\cos \alpha|$ (or $|\cos \alpha^*|$) < 1.0.

[2]The general helix-screw symmetry operation is not an allowed element of a crystallographic group, so that the molecular environment of the transformed unit will not in general be identical to that of the untransformed unit (unless the crystal is considered to be one dimensional). This input is simply an expedient for use in plotting helical polymer structure models with minimum input. In general it would be possible to produce the same results by specifying the *complete crystallographic asymmetric unit* and normal crystallographic symmetry transformations.

[3]This input mode is only meaningful if the cell angles α and β are 90°, so that **c** lies along **c*** and the helix can continue uninterrupted from cell to cell along the **c** axis.

(third axis of the standard Cartesian system; see 3.1.8). The two symmetry types can be intermixed if desired.

Columns	(*a*) Crystallographic symmetry (70–72 $\leqq$ 5)	(*b*) Helix symmetry (70–72 $\geqq$ 5)
1	$\neq 0$ last card only	$\neq 0$ last card only
2–15	T_1	T_1
16–18	S_{11}	–
19–21	S_{12}	–
22–24	S_{13}	–
25–39	T_2	T_2
40–42	S_{21}	–
43–45	S_{22}	–
46–48	S_{23}	–
49–63	T_3	T_3
64–66	S_{31}	L
67–69	S_{32}	M
70–72	S_{33}	N

(*a*) Crystallographic symmetry: Transformed triclinic coordinates (X_1, Y_1, Z_1) are obtained from input triclinic coordinates (X, Y, Z) by

$$X_1 = T_1 + S_{11} X + S_{12} Y + S_{13} Z ,$$
$$Y_1 = T_2 + S_{21} X + S_{22} Y + S_{23} Z ,$$
$$Z_1 = T_3 + S_{31} X + S_{32} Y + S_{33} Z ,$$

or in matrix notation

$$\mathbf{X}_1 = \mathbf{T} + \mathbf{S}\,\mathbf{X} ,$$

where

$\mathbf{T} = (T_1, T_2, T_3)$ as fractions of cell edges.

(*b*) Helix screw symmetry:

$$\mathbf{X}_1 = \mathbf{T} + \mathbf{S}\,\mathbf{X} ,$$

where

$\mathbf{T} = (T_1,\ T_2,\ T_3 + L/N)$ as fractions of cell edge and

$\mathbf{S}$ = a counterclockwise rotation of $L{\cdot}M/N$ cycles about c* axis.

For example, the Pauling and Corey right-handed alpha helix repeats after 5 turns and 18 residues and can be represented by 18 symmetry cards with $N = 18$; $M = 5$; $L = 0, 1, \ldots, 17$; $T_1, T_2, T_3 = 0$. The input atom list contains the contents of one residue.

3.2.4 Atom Parameter Cards (1 $\leqq$ NATOM $\leqq$ 200). – Two cards are required for each input atom. The first contains the chemical symbol and positional parameters, and the second contains temperature factor

information or other information which specifies how the atom is to be represented on the drawing. The format allows the use of the atom parameter cards produced by the FORTRAN Least Squares Program OR FLS by Busing, Martin, and Levy (1962).[4] Several alternate inputs are possible for each of the two cards, and the number in columns 55–63 denotes the type used on that particular card.

3.2.4.1 Positional Parameter Card. – FORMAT(A6,3X,5F9.6,F9.0)

Columns				
1–6	Up to six alphanumeric characters centered in the six-place field			
7–9	Blank			
	Type 0	Type 1	Type 2	Type 3
10–18	–	–	–	x_0 (A) Cartesian
19–27	–	–	–	y_0 (A) Cartesian
28–36	x (fractional, crystal)	x (A, crystal)	x (A, Cartesian)	r (A) cylindrical
37–45	y (fractional, crystal)	y (A, crystal)	y (A, Cartesian)	ϕ (°) cylindrical
46–54	z (fractional, crystal)	z (A, crystal)	z (A, Cartesian)	z (A) cylindrical
55–63	0 or blank	1	2	3

Type 0 is the normal input based on triclinic coordinates. Some authors give coordinates in A along the unit cell vector; type 1 would be used in such a case. Type 2 allows one to place a model described in Cartesian coordinates onto a general triclinic lattice. The orientation of the Cartesian system $x\ y\ z$ in the general lattice **a b c** is the standard type described in 3.1.8 with x along **a** and z along **c***. Type 3 is similar to type 2 except that cylindrical coordinates r, ϕ, z are used and the axis of the system can be displaced from zero in the $x\ y$ Cartesian plane by the displacement x_0, y_0. Cylindrical coordinates are often used in the literature to describe a helical structure. The x_0, y_0 translation should be zero if helical symmetry operators are used. This translation feature is meant to be used in explicitly describing the contents of a multiple helix cell.

3.2.4.2 Temperature Factor Card. – FORMAT(I1,F8.6,5F9.6,F9.0)

Columns						
1	A sentinel $\neq 0$ for last atom only					
	Type 0,1,2,3	Type 4,5	Type 6		Type 7	
2–9	b_{11}	U_{11}	B	B	R	R
10–18	b_{22}	U_{22}	0	0	0	0
19–27	b_{33}	U_{33}	0	$\}$ [VDC$_1$]	0	$\}$ [VDC$_1$]
28–36	b_{12}	U_{12}	0		0	
37–45	b_{13}	U_{13}	0	$\}$ [VDC$_2$]	0	$\}$ [VDC$_2$]
46–54	b_{23}	U_{23}	0		0	
55–63	0,1,2,3	4,5	6 (or 0)	6 (or 0)	7	7

[4]W. R. Busing and H. A. Levy, *A Fortran Crystallographic Least-Squares Program*, ORNL-TM-305 (Nov. 21, 1962).

The coefficients b_{ij} $(i,j = 1,2,3)$ of the anisotropic temperature factor, types 0–3, are defined as follows: The complete temperature factor is

$$(\text{Base})^{\{-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + C\, b_{12}hk + C\, b_{13}hl + C\, b_{23}kl)\}}$$

where in type 0: Base = e, C = 2;

type 1: Base = e, C = 1;

type 2: Base = 2, C = 2;

type 3: Base = 2, C = 1.

The coefficients $U_{ij}(i,j = 1,2,3)$ of the anisotropic temperature factor, types 4 and 5, are defined as follows: The complete temperature factor is

$$\exp\left\{-\frac{1}{4}\left(\mathbf{a}_1^{*2}U_{11}h^2 + \mathbf{a}_2^{*2}U_{22}k^2 + \mathbf{a}_3^{*2}U_{33}l^2 + C\mathbf{a}_1^*\mathbf{a}_2^*U_{12}hk + C\mathbf{a}_1^*\mathbf{a}_3^*U_{13}hl + C\mathbf{a}_2^*\mathbf{a}_3^*U_{23}kl\right)\right\},$$

where $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ are reciprocal cell dimensions and in type 4, C = 2; in type 5, C = 1. Type 6 allows the input of the Debye-Waller isotropic temperature factor B, which is used as follows:

$$\exp\left(-B \sin^2 \theta/\lambda^2\right),$$

where λ is the wavelength and θ is the Bragg angle. The parameter B is related to mean-square displacement $\overline{\mu^2}$ of the atom from its mean position by the relation

$$B = 8\pi^2\, \overline{\mu^2}\,.$$

When the isotropic temperature factor is used, the atom is represented as an isotropic ellipsoid (sphere) with equal principal axes of length μ. When the field in columns 19–27 is 0 or blank, the directions of the principal axes are along the standard Cartesian system axes (see 3.1.8). However, one can reorient these arbitary orthogonal vectors by using the two vector designator codes VDC_1 and VDC_2; then the three new principal-axis vectors will be VDC_1, $(\text{VDC}_1 \times \text{VDC}_2)$, and $\text{VDC}_1 \times (\text{VDC}_1 \times \text{VDC}_2)$. This is strictly an artistic feature of no physical significance.

Type 7 allows the input of arbitrary spheres of radius $\overline{\mu} = R$ in angstroms. The vector triplet orientation is specified as with type 6. An additional feature allows one to use a completely blank card (except perhaps column 1) for a temperature factor card. In this case the program assumes type 7 with an R = 0.1 A.

3.3 Instruction Input

The instructions are the commands used in programming an illustration, and there is no required sequence for the instructions, except as indicated by the programming logic. Some instructions require trailer cards, which may have three different formats. The program is informed what the format of the next card will be with the "look ahead" field, columns 1 to 3. The program action is also influenced by this information.

"Look ahead" (columns 1–3)	Next card will be –	Program action
0 or blank	Format No. 0, a new instruction	Execute present instruction; then read next card.
1	Format No. 1, continuation of present instruction	Read continuation card; then check "Look ahead."
2	Format No. 2, vector search code	Read (VSC) card; then check "Look ahead."
3	Format No. 3, alphanumeric info.	Read alphanumeric info. and execute instruction; then read next card.

3.3.1 Instruction Cards. – *3.3.1.1 The Format No. 0 Instruction Card.* – FORMAT(I3,I6,7F9.0)

Columns	
1–3	"Look ahead" (0,1,2,3)
4–9	Instruction number
10–18	1st parameter
19–27	2nd parameter
.	.
.	.
.	.
64–72	7th parameter

3.3.1.2 Format No. 1, Instruction Continuation Card. – FORMAT(I3,I6,7F9.0) A maximum of 19 continuation cards per instruction is permitted.

Columns	
1–3	"Look ahead" (0,1,2,3)
4–9	Blank
10–18	8th parameter, or 15th, . . . , or 134th
.	.
.	.
.	.
64–72	14th parameter, or 21st, . . . , or 140th

3.3.1.3 Format No. 2, Vector Search Code (VSC) Card. – FORMAT(I3,6X,5I3,8F6.0) A maximum of twenty VSC cards is allowed. These cards can be entered with any instruction, but only certain instructions will use them. They must be entered with the particular instructions that require them; that is, they are not held over. Table 3.1 will be referred to as the individual instructions are explained.

Table 3.1. Vector Search Code Cards

Columns	Search Instructions 101 402 102 412	Bond Plotting Instructions 801	802	803
1–3	Look ahead	Look ahead	Look ahead	Look ahead
4–9	–	–	–	–
10–12	ORG. ANR	–	ANR (A)	ANR (A)
13–15		–		
16–18	TAR. ANR	–	ANR (B)	ANR (B)
19–21		–		
22–24	–	Bond type	Bond type	–
25–30	*D* min (A)	–	*D* min (A)	*D* min (A)
31–36	*D* max (A)	–	*D* max (A)	*D* max (A)
37–42	–	Bond radius (A)	Bond radius (A)	–
43–48	–	Perspective label hgt. (in.)	Perspective label hgt. (in.)	–
49–54	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–
55–60	–	Nonperspective label hgt. (in.)	Nonperspective label hgt. (in.)	–
61–66	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–
67–72	–	Digits indicator	Digits indicator	–

3.3.1.4 Format No. 3, Labeling Card. – FORMAT(12A6)

Columns

1–72 Up to 72 digits of alphanumeric label information centered about columns 36 and 37. Note: There is no "look ahead" column in Format No. 3; the next card must be a new instruction card. Instructions 902, 903, and 913 are the only ones which require this input. It may be used with other instructions as a device to transfer comments about the particular instruction to the monitor output listing.

3.3.2 Structure Analysis Instructions (100 Series). – This series of instructions is not connected with drawing illustrations. It is used to obtain on the standard output medium of the computer a convenient tabulation of the chemically interesting aspects of a crystal structure, such as interatomic distances, interatomic angles, and principal axes of thermal motion.

3.3.2.1 Instructions 101 and 102. – These instructions call subroutine SEARCH, which finds all "target" atoms within a sphere of enclosure of radius *D* max about a particular "origin" atom. The instruction card has an atom number run (see 3.1.4) of origin atoms (Org. ANR) and an atom number run of target atoms (Tar. ANR). The Org. ANR allows one to calculate several spheres successively with a printout of results after each one. For example, suppose there are nine atoms in the input list

and we want the total surroundings of atoms 365502, 465502, and 565502 out to a maximum radius, *D* max, of 4 A. The Org. ANR is designated (365502, 5) or (365502, 565502)[5] and the Tar. ANR is designated (1,9). Further selection of the interatomic vectors from a particular origin atom to the target atoms which fall within the limiting sphere is possible with vector search code (VSC) cards of Format No. 2 (see 3.3.1), which can be entered with the instruction. If VSC cards are present, then the vectors must also satisfy one of the VSC's in order to be saved. A VSC card to specify the selection of a shell of vectors in the above example might be coded as follows: Org. ANR (3,5) Tar. ANR (1,9) Dist. range (2.0, 2.7). More selective VSC's are also possible. They are meant to be based on known interatomic distance ranges, such as those tabulated in Vol. III of the *International Tables for X-Ray Crystallography.*[6]

Vectors found about a particular origin atom are stored in a table of dimension 200 sorted on distance. Duplicate vectors (not duplicate distances) are eliminated. If more than 200 acceptable atoms are found about an origin atom, the 200 shortest vectors are saved. At the end of the search about each origin atom, the distances are printed out along with the atom designator codes (ADC), chemical symbols, and triclinic crystal coordinates for the origin and target atoms. If the instruction is 102, all possible interatomic angles are also calculated and printed for the stored vectors. There will be $n(n-1)/2$ angles for n vectors.

The tabulation of atom designator codes, which is obtained automatically when these instructions are given, is often useful for planning an illustration. Although the tabulation is complete within the addressable region of 9^3 cells, the computing time is generally only a matter of seconds per sphere unless a very large *D* max is specified. Subroutine SEARCH is a rather elaborate routine designed to minimize computing time. This subroutine is also used for instructions 402 and 403, which are explained in 3.3.4.

Instruction card for instructions 101 and 102:

Columns	
1–3	0 or 2 (look ahead)
4–9	101 or 102
10–18, 19–27	ORIGIN (atom number run)
28–36, 37–45	TARGET (atom number run)
46–54	*D* max (A)

3.3.2.2 Instruction 103. – Principal axes of thermal motion (or arbitrary spheres, according to the temperature factor input) for all atoms in the input list are calculated. The printout contains root-mean-

[5]For the origin sequence 355501, 455501, 555501, an Org. ANR input (3,5) is allowed as well as (355501,5) and (355501,555501); however, the Tar. ANR must always be designated as shown. In sect. 2.1, Org. ANR is designated as ORG 1, ORG 2; and Tar. ANR is denoted by TAR 1, TAR 2.

[6]H. Ondik and D. Smith, "Interatomic Distances in Inorganic Compounds," p. 257 in *International Tables for X-Ray Crystallography*, vol. III, ed. by K. Lonsdale, Kynoch, Birmingham, 1962.

square amplitudes of displacement along the principal axes of the trivariate normal probability density function and direction cosines for the principal axes relative to the reference Cartesian base vectors. A symmetric covariance dispersion matrix based on the reference Cartesian system is also printed out. The diagonal elements are the mean-square displacements along the reference Cartesian axes.

Columns

1–3	0 or blank (look ahead)
3–9	Blank
10–18	103

3.3.3 Plotter Control Instructions (200 Series). – The 200 series is a group of instructions that control the plotter initialization, frame advance, termination, and any other peripheral commands that are required for a particular equipment configuration or plotting package. When the program is modified for a different equipment configuration, these series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements. Instructions for controlling the CalComp 580 off-line magnetic tape plotting system[7] are given here.

3.3.3.1 Instruction 201, Plot Package Initialization. – This instruction must be executed before any plotting can take place. It is a safe policy always to make this the first instruction card. It should be used only once per computer job regardless of how many plots are to be drawn during the job.

3.3.3.2 Instruction 202, Plot Terminate and Frame Advance. – This takes care of putting the correct plot termination information onto the magnetic tape to inform the plotter that the current plot is finished. It also allows advance of the paper so that the old plot is removed and new paper is in position for the next plot.

Columns	Instruction 201	Instruction 202
1–3	Blank	Blank
4–9	201	202
10–18	–	Plotter movement along x edge of paper in inches

3.3.4 Plot Boundary Instructions (300 Series). – This is a set of miscellaneous instructions for specifying the dimensions of the drawing, viewing distance, general lettering orientation, and pen displacement for line retracing.

3.3.4.1 Instruction 301. – This instruction defines the limiting x and y dimensions, in inches, of the plot boundary and the border indentations. The boundary dimensions must not exceed those allowed by the plotter. The program will prevent the pen from getting closer than 0.1 in. to any boundary. The border indentation is an equal margin inside the entire boundary. When automatic scaling is used (600

[7]The CalComp is an incremental plotter. The particular Benson-Lehner model available at Oak Ridge Central Data Processing Facility has also been used. The Benson-Lehner is an electromechanical x-y plotter with an analog converter. In general it seems that an incremental plotter is better suited to the requirement of OR TEP. The user should be warned that in the author's experience the magnetic tape plotting systems are notoriously troublesome; an annoying percentage of plot failures is to be expected because of equipment malfunctions.

series), the center points of the atoms are prevented from falling in the margin; but the atom representation, which has a finite size, may extend into that area. To compensate for the overlap, the border dimensions should be large when the overall drawing scale and the ellipsoid scale are expected to be large.

In addition, instruction 301 specifies the perspective viewing distance, in inches, from the plane of the drawing. An entry of 0 for view distance is used to indicate an infinite view distance, and the crystal structure is then mapped in parallel projection normal to the drawing board.

Columns		Primer Constant
1–3	–	–
4–9	301	–
10–18	Plot x limit (in inches)	30.
19–27	Plot y limit (in inches)	11.
28–36	View distance (in inches)	0. (parallel proj.)
37–45	Border (in inches)	0.5

3.3.4.2 Instruction 302, Title Rotation. – For regular titles and chemical symbols, the title rotation is specified with instruction 302. The lettering base line for all lettering is rotated counterclockwise by an angle theta, in degrees, from the x axis of the plotter. Although any value is allowed, 0° and –90° are the values most often used, so that, when one views the finished drawing, either the y plotter axis is vertical or the x plotter axis is vertical.

Columns		Primer Constant
1–3	Blank	–
4–9	302	–
10–18	Theta in degrees	0.

3.3.4.3 Instruction 303, Retrace Displacement. – For artistic purposes, certain lines are made heavier than others by retracing over the path several times with slight pen displacements (DISP) from the original path. For example, in drawing ellipsoids the forward half of the principal plane trace is made heavier than the hidden half so the eye does not confuse the two halves. In addition all regular lettering (but not perspective lettering) is gone over four times to give it boldface appearance. In preliminary runs or when the plotter is not of the incremental type, this embellishment may be objectionable to the user because of the increased computing and plotting times (particularly the latter). All retracing can be eliminated by setting DISP = 0. The primer parameter for DISP is 0.005 in., which is the resolution of the CalComp plotters at ORNL. For other plotters or for various inking pen sizes, DISP can be reset at the user's discretion.

Columns		Primer Constant
1–3	–	–
4–9	303	–
10–18	DISP (in inches)	0.005

3.3.5 Atom List Instructions (400 Series). – This series allows the user to specify which atoms are to be included in the illustration. The atom designators for the chosen atoms are stored in the ATOMS array for future use by other instructions. The ATOMS array can hold 500 atoms; but if the intended illustration has more than this, the illustration can be segmented and the segments drawn sequentially on the same plot. This technique may also be used when different parts of the drawing are to have different graphic representations. That is, we would define the first segment, draw it with the first representation, clear the ATOMS array, define the second segment, and draw it with the second graphic representation.

Groups of atoms are added to or eliminated from the ATOMS array (which is set to zero at the start of the program) with the 400 and 410 series respectively. The groups can be denoted by atom designator runs (see 3.1.3), spheres of atoms about any center point (see 3.1.6), and rectangular boxes of atoms centered on any point (see 3.1.7). Duplicate entries of the same atomic position are prevented by the program. The content of the ATOMS list is printed on the monitor output tape after each 400 series instruction.

3.3.5.1 Instructions 401 and 411, Atom Designator Run Add and Atom Designator Run Eliminate. – These instructions can contain: (*a*) atom designator codes (ADC) for a single atom, (*b*) atom designator runs (ADR) for several atoms in a run, (c) blank fields (except between the two entries of a run), and (*d*) any combinations of (*a*), (*b*), and (*c*). Since up to 19 Format No. 1 continuations are possible per instruction, up to 70 runs can be made per instruction and an unlimited number of instructions can be used. The ATOMS list, however, will only accept the first 500 atoms.

Columns	
1–3	Blank or 1 (depending on what follows)
4–9	401 or 411
10–18	As described above
.	
.	
.	
64–72	

3.3.5.2 Instructions 402 and 412, Sphere of Enclosure Add and Sphere of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete, partial, or vector screened, see 3.1.6) of a sphere of enclosure about any addressable point. For instruction 402, the contents of the spheres are *added to* the atom list except for positional duplications, which are omitted. In the 412 instructions, all points in the spheres are *eliminated from* the atoms list if they are present in that list. The instructions call subroutine SEARCH, and the instruction input details are identical to those of instructions 101 and 102 (see 3.3.2.1) except for the instruction number. In the monitor output, only the ATOMS list atom designator codes are printed and not the coordinates and interatomic distances. If the origin atoms on which the spheres of enclosure are centered are to be saved, the target atom number run (Tar. ANR) must contain this atom number. Furthermore, if vector

search code cards of Format No. 2 are used, one of them must satisfy the intra-atom null vector for the origin atom in order to retain it.

3.3.5.3 Instructions 403 and 413, Box of Enclosure Add and Box of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete or partial but *not* vector screened, see 3.1.7) of a box of enclosure about any addressable point (or atom number run of addressable points). The three axes of the box are parallel to the three base vectors of the reference Cartesian system, and the *semidimensions* of the box are specified on the instruction card. If an orientation of the box different from the standard orientation (see 3.1.8) is desired, than a 501 or a 502 instruction, or both, should be used before this instruction to reorient the reference Cartesian system. After this instruction has been executed, the reference system can undergo further reorientation as desired for plotting purposes, etc.

As in the case of the sphere of enclosure (see 3.3.5.2), the origin atom on which the box is centered will not be included unless the target atom number run includes the origin atom number. Vector search codes are not used by this instruction. Subroutine SEARCH is used by this instruction, and the instruction input details are similar to those described in 3.3.2.1 except that D max is replaced by the semidimension $a/2$ of the box and the following fields on the card are used to specify the other two semidimensions $b/2$ and $c/2$. One must use caution in choosing the box dimensions so that the atom table does not overflow.

Columns	
1–3	Blank
6–9	403 (or 413)
10–18	Origin ANR (see 3.3.2.1)
19–27	
28–36	Target ANR (see 3.3.2.1)
37–45	
46–54	$a/2$
55–63	$b/2$
64–72	$c/2$

3.3.5.4 Instruction 410, Clear Atoms List. – This instruction clears the atoms list to zero. When the program is first entered the list is automatically set to zero.

3.3.6 Orienting Instructions (500 Series). – This series of instructions orients the reference and working Cartesian systems (see 3.1.8). Each time the reference system is redefined with a 501 or rotated with a 502, the working system is automatically made coincident with the reference system. The working system can be displaced from the reference system by rotating about an axis of the reference system with a 503 instruction. The working system is always positioned by a rotation from the reference system and does not depend on the previous working system orientation. After each 500 series instruction, the base vectors of the relevant Cartesian system are printed out. These vectors are based on the triclinic coordinate system. The postfactor transformation matrix for converting from triclinic coordinates to

Cartesian coordinates is also printed out. The inverse transformation matrix may be formed by placing the three base vectors together in row vector form.

3.3.6.1 Instruction 501, Reference Cartesian System Assignment. – Any Cartesian coordinate system is based on three orthonormal base vectors and an origin point. The origin point in the model (ORGN) is specified with an atom designator code. The three orthonormal base vectors can be described by two non-collinear vectors, and OR TEP provides the two following separate techniques for performing this operation, using vector cross products of the two vectors **u** and **v**.

	Type A	Type B
Base vector 1 (x axis)	**u**	**u**
Base vector 2 (y axis)	**u** × **v**	(**u** × **v**) × **u**
Base vector 3 (z axis)	**u** × (**u** × **v**)	**u** × **v**

The reference system x and y axes will parallel the plotter x and y axes, and the origin point ORGN will lie in the plane of the plotter. The viewer will be looking into the z axis vector of the coordinate system from a distance VIEW in inches (see 3.3.4.1) directly above the origin point.

Columns		Effective Primer Constant
1–3	–	–
6–9	501	–
10–18	ORGN(ADC)	055500
19–27	Vector **u** (VDC)	055500
28–36		065500
37–45	Vector **v** (VDC)	055500
46–54		056500
55–63	–	–
64–72	0 = Type A, >0 = Type B	1

3.3.6.2 Instruction 502, Reference Cartesian System Rotation. – The crystal model can be given any orientation desired with a series of rotations of the model about the reference system axes. In general, three rotations (e.g., those of an Eulerian system) are sufficient to achieve any orientation, but for convenience an unlimited number of rotations are permitted in the program. In addition, rotations of 120° about the body diagonal of the reference Cartesian system are permitted (this is achieved by a cyclic permutation of reference base vectors).

Each operation requires two fields in the instruction card. For axial rotations, the first field of each pair will have the number 1, 2, or 3 to indicate rotation about the x, y, or z axes of the reference system. The second field will have the rotation angle in degrees for a right-handed rotation of the model about the designated axis (i.e., a positive angle signifies a counterclockwise rotation of the structure with the designated axis pointing toward the reader). The body diagonal rotation is designated by either a (– 1)

or a (−2) in the first field to indicate a 120° or a 240° right-handed rotation about the body diagonal, and the second field is blank. A (−3) would rotate the structure completely around and thus not change its previous orientation.

Columns	
	First Card
1–3	0 (or 1 if continued on next card)
4–9	502
10–18	1,2,3,−1,−2
19–27	ϕ_1°
28–36	1,2,3,−1,−2
37–45	ϕ_2°
46–54	1,2,3,−1,−2
55–63	ϕ_3°
64–72	1,2,3,−1,−2
	Second Card
10–18	ϕ_4°
.	
.	
.	

If desired, each rotation can be executed with a separate 502 instruction card.

3.3.6.3 Instruction 503, Working Cartesian System Rotation (Stereoscopic Rotation). – The working (minor) Cartesian system is automatically made coincident with the reference system whenever the reference system is redefined with a 501 instruction or rotated with a 502 instruction. To define an orientation of the working system which is not coincident with the reference system we use a 503 instruction, which allows one rotation about one axis of the reference system. Actually any number of successive rotations can be made, but the effect is not cumulative since the starting point for each rotation is always the reference system. Body diagonal rotations are not permitted.

A 503 rotation normally precedes each member of a stereoscopic pair of plots. The rotation is about axis 2 if the stereo pair is to be viewed with the x axis parallel to the observer's interocular line and about axis 1 if the *y* axis is to be parallel to that line.

Column	
1–3	–
4–9	503
10–18	1,2,3
19–27	ω°

3.3.7 Positioning and Scaling Instructions (600 Series). – These instructions are used to direct the placement of the origin point ORGN (specified by instruction 501) onto the drawing (dimensioned by in-

struction 301). In addition the three-dimensional assembly of atoms (chosen by the 400 series instruction) constituting the model is scaled. The atomic centers of the model will then be hanging in space above and below the drawing board correctly positioned to be projected from the eye point described with 301.

3.3.7.1 Normal Modes of Positioning and Scaling. – Several normal modes of operation are available to the user for positioning and scaling the model. Instruction 601 requires the user to supply a complete explicit description of position (x_0, y_0) and scale (SCAL1). At the other extreme, instruction 604 automatically scales and positions the model so that the peripheral projected atom centers will touch two opposite borders and the peripheral atoms in the remaining dimensions will be centered on the drawing. An intermediate mode is available through 602, which provides automatic scaling after explicit positioning. In general this allows only one edge of the model to touch a border. Finally, instruction 603 requires an explicit scale and does automatic centering.

In general the 604 is the easiest and safest one to use, but situations arise in which the user should not relinquish control to the program. For example, if a big illustration is to be drawn piecewise on a small plotter, the user will have to maintain control over the scale, and probably over positioning, so that the partial plots can be fitted together correctly.

A second scale factor SCAL2 is required in connection with the ellipsoid (or sphere) size. It is a dimensionless scale factor ratio used to modify all rms displacement values before plotting equiprobability ellipsoids or spheres. A table of SCAL2 values vs probability is given in Sect. 5.2. The primer constant for SCAL2 is 1.54, corresponding to 50% probability. If the instruction's entry for SCAL2 is 0 or blank, then SCAL2 is not modified by the instruction. The same statement also holds for x_0, y_0, and SCAL1. That is, if the instruction entry is zero or blank for any of these, then the value of the constant in memory is not changed. This means that an x_0 or y_0 cannot be entered as exactly zero, so that if, zero is wanted, a small nonzero number should be entered.

Columns	601	602	603	604	Primer Constant
1–3	–	–	–	–	–
4–9	601	602	603	604	–
10–18	x_0	x_0	–	–	15.0
19–27	y_0	y_0	–	–	5.5
28–36	SCAL1	–	SCAL1	–	1.0
37–45	SCAL2	SCAL2	SCAL2	SCAL2	1.54

3.3.7.2 Incremental Modes of Positioning and Scaling. – Additional flexibility is provided through the incremental instructions 611, 612, and 613. These allow the user to "nudge" the model or modify the scale factor (SCAL1), or both, after the parameters have been initially set with a previous 600 series instruction. The 611 instruction adds Δx_0, Δy_0 to the previous x_0, y_0 position for the ORGN placement and multiplies the existing SCAL1 by ΔK (except if $\Delta K = 0$, SCAL1 is unmodified). Instruction 612 increments the position and then does an automatic scaling; 613 first increments the scale (by multiplying by ΔK) and then automatically repositions.

A conservative general approach is to follow a 604 with a 611 having $\Delta x_0 = 0$, $\Delta y_0 = 0$ and $\Delta K = 0.9$. This will simply reduce the scale 10% so that there is more space for labels, etc.

Column	611	612	613
1–3	–	–	–
4–9	611	612	613
10–18	Δx_0	Δx_0	–
19–27	Δy_0	Δy_0	–
28–36	ΔK	–	ΔK
37–45	SCAL2	SCAL2	SCAL2

3.3.8 Atom Plotting Instructions (700 Series). – These instructions are concerned with drawing various representations of the atom based on the familiar ball-and-stick molecular model. The ball in the general case is an ellipsoid representing a contour surface of equal probability density. Alternatively, when thermal motion is not being portrayed, the ball can be a sphere of arbitrary dimension. The 700 series also has provision for labeling the atomic site with the corresponding chemical symbol. The instructions in this series draw the "ATOMS list" atoms which project onto the usable part of the drawing area. Atoms found to be out of bounds are bypassed, and a Fault Message (NG = 10) is printed on the monitor output. An atom is out of bounds under the following conditions: (1) if its z coordinate in the scaled reference Cartesian system is greater than $\frac{1}{2}$ the viewing distance, (2) if its center after projection falls outside the limiting boundary of the drawing board, or (3) if the projected center is within $\frac{3}{4}$ of the margin width (BRDR) of a limiting boundary.

An ellipsoid, for graphical purposes in OR TEP, is considered to be composed of ellipses and straight lines. The ellipses are of two types, principal ellipses and boundary ellipses. Relative to the viewpoint, a principal ellipse is further subdivided into a front half and a back, or hidden, half. There are three principal ellipses per ellipsoid, corresponding to the three principal planes. The boundary ellipse is the edge of the ellipsoid as seen from the viewpont. The front and back halves of the principal ellipses meet at the boundary ellipse. The straight-line segments of the OR TEP ellipsoid are the forward principal axes, reverse principal axes, and octant shading lines.

Figure 3.1 shows various combinations of these elements. It is obvious that certain of these combinations are better representations than others. Instruction 701 generates the 5A model of Fig. 3.1, instruction 702 generates 2A, and 703 produces 3B. Instruction 704 draws the boundary ellipse alone. If an atom is entered as a sphere, the boundary will be circular before projection and slightly elliptical after perspective projection. Instruction 705 allows the user to make up any representation from the basic components.

Chemical symbols up to six alphanumeric characters in length are included with the input structural parameters for each atom. These symbols can be put onto the illustration with one 700 series or several 900 series instructions. The 700 series places the center of the six-character field of each atom in the same position relative to the atom center; the 900 series allows the user to position each symbol individually. The 700 series requires only three parameters as follows: (1) symbol height in inches, (2) parallel

(left-right) offset in inches, and (3) perpendicular (up-down) offset in inches. The parameters refer to the model before projection, and they will change slightly during perspective projection. The parallel and perpendicular offset refer to the exact center of the six-character input field and are relative to the lettering base line set up with the 302 theta rotation. A symbol height of 0 or blank will cause the symbol-drawing routine to be bypassed.

It is possible to vary the thickness of the boundary ellipse line by making it a function of z, the height of the atom from the drawing board. This option is normally used with the 704 (boundary only)

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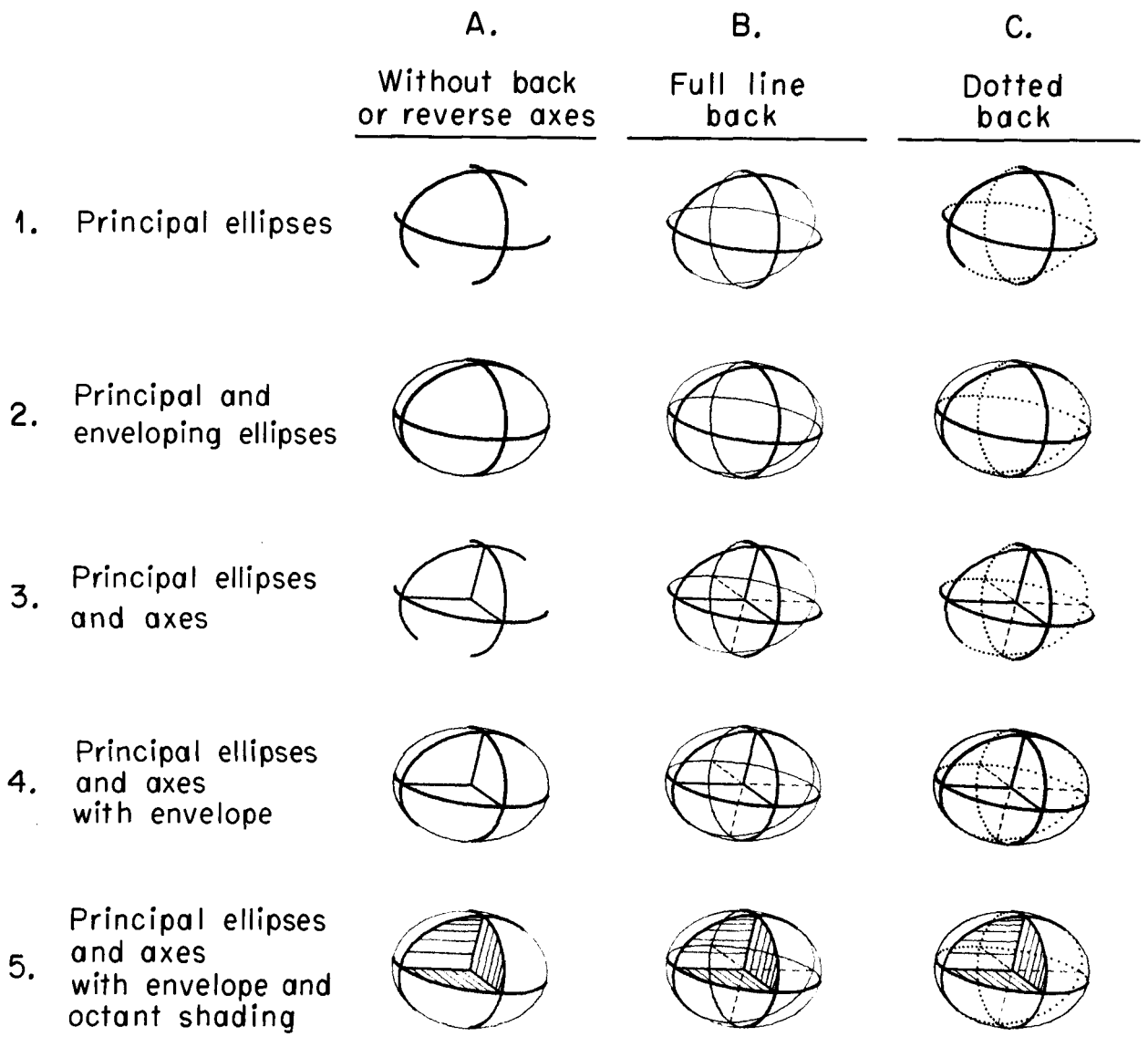

Fig. 3.1. Various Combinations of Ellipsoid Components.

instruction but will work for any 700 instruction. Entries are put in the A_0 and A_1 fields of the instruction continuation card to specify the coefficients of

$$\Delta R(z) = A_0 + A_1 z ,$$

where

ΔR is the increase in radial dimension to be added to the width of the single pen line,

A_0 is ΔR for an atom at $z = 0$, and

A_1 is the rate of increase in radial dimension with z.

As an example, assume that the atoms of the scaled model range from 5 in. below to 5 in. above the drawing board and the pen width is 0.2 mm (.008 in.). If we want the closest ellipse boundary to be five times as wide as the farthest, then $\Delta R(-5 \text{ in.}) = 0$, $\Delta R(5) = 0.008 \times (5 - 1) = 0.032$ in.; thus $A_0 = 0.016$ in. and $A_1 = 0.0032$ in.

The program widens the line by stepping radially in increments of DISP, which is set by primer constant to 0.005 in. A 303 instruction can be used to change DISP if desired.

The monitor output for the 701 through 705 instructions consists of the following:

1. x,y plotter coordinates: the coordinates, in inches, for the projected atom center on the plot, measured from the lower left-hand corner of the limiting boundary. This is the fixed plotter coordinate system with origin point set by the plotter operator.

2. x,y,z working Cartesian coordinates: the coordinates, in inches, for the oriented and scaled atomic model before projection. The x and y axes parallel the plotter x and y axes, and the origin of the system is in the plane of the plotter at the point x_0,y_0 (see 3.3.7) in plotter coordinates. The point ORGN of the scaled model is at this point (see 3.3.6.1).

3. x,y,z triclinic coordinates, in fractions of the unit-cell edges relative to the crystal unit-cell origin.

4. Principal axes of thermal motion, consisting of (*a*) principal values of root-mean-square displacement and (*b*) direction cosine for principal vectors relative to the working Cartesian system.

5. The atom designator code and chemical symbol for the atom.

Instructions 711 through 715 are identical to 701 through 705 except that *the 710 series suppresses all monitor output except fault messages.*

3.3.8.1 Atom Plotting Instructions 701, 702, 703, 704, and 711, 712, 713, 714. –

Columns	First Card
1–3	1 (if boundary retracing is desired; otherwise 0)
4–9	701, 702, 703, 704, 711, 712, 713, 714
10–18	Blank
19–27	Blank
28–36	Blank
37–45	Blank

46–54	Symbol height (in.)
55–63	Perpendicular offset (in.)
64–72	Parallel offset (in.)

Second Card (needed only for boundary retracing)

1–3	Blank
4–9	Blank
10–18	A_0 (in.)
19–27	A_1 (in.)

3.3.8.2 Atom Plotting Instructions 705 and 715. –

Columns

First Card

1–3	1 (if boundary retracing is desired; otherwise 0)
4–9	705 or 715
10–18	NPLANE = 0, no ellipsoid components = 1, boundary ellipse only = 3, principal ellipses only = 4, boundary + principal ellipses
19–27	NDOT (back side of principal ellipses) <0, solid line back side = 0, back side omitted = 3, 4 dots on back side = 4, 8 dots on back side = 5, 16 dots on back side = 6, 32 dots on back side
28–36	NLINE (forward principal axes and shading) = 0, no forward axes or shading = 1, forward principal axes only = N, forward axes + (N – 1) line shading
37–45	NDASH (dashed reverse principal axes) = 0, no reverse axes = N, dashed reverse axes with N dashes
46–54	Symbol height (in.)
55–63	Perpendicular offset (in.) } for symbols
64–72	Parallel offset (in.) } for symbols

Second Card same as 701

3.3.9 Bond Plotting Instructions (800 Series). – The bond plotting instructions are grouped into two general types, explicit and implicit, depending on how the bonds are specified. Explicit bonds require a vector designator code (see 3.1.2) for each bond. Implicit bonds make use of vector search codes (see 3.1.5) to find pairs of atoms from the ATOMS array set up by the 400 series instructions.

There are two types of bonds that can be drawn, stick bonds and line bonds. The line bond is a very crude, but rapid, method useful in drawing preliminary illustrations. It is constructed by placing centered symbols (e.g., +, ×, *, etc.) on the two atom sites and drawing a single straight line between them. Line bonds are always specified implicitly (803, 813 instructions).

The more elaborate bond is the stick bond, which could also be called a conical bond because of its accentuated perspective taper.[8] Each end of the bond intersects either (1) an ellipsoid or (2) an enveloping cone (tangent cone) which has its apex at the viewpoint and is tangent to an ellipsoid. In general, the ellipsoid intersection is automatically used if the axis of the bond intersects the ellipsoid at a point which is visible to the viewpoint; otherwise, the tangent cone intersection is used, so that the bond appears to terminate at the boundary of the ellipsoid. However, the user can specify that the ellipsoid intersection always be used in order to make the skeleton type model (e.g., 3B of Fig. 3.1) appear even more transparent. The radius of the stick bond and the number of lines which are used to draw the bond are specified by input parameters.

Bond-distance labels can be drawn automatically with stick bonds, but not with line bonds. The bond-distance label numbers are in Angstrom units to one, two, or three places past the decimal point. The bond labels on the illustration will have their base lines parallel to the stick bonds and will be right side up for the viewer. The height of the label in inches and the perpendicular offset distance for the center of the label relative to the center of the bond are parameters to be specified by the user. With the present primer constant for FORE, if the sine of the angle between the bond and the mean viewing vector is greater than 0.5, the lettering is done in perspective along the bond. When the sine of the angle is less than 0.5, the perspective lettering would be excessively foreshortened. The lettering is then made parallel to the plane of the drawing with its base line parallel to the projected bond. Different lettering heights and different perpendicular offset distances can be assigned to the perspective and nonperspective bond-distance labels.

All bond parameters are input with Format No. 2 trailer cards (see 3.3.1). The bond parameters are as follows:

1. Bond type (for stick bond) is designated by an integer NBOND, where $-5 \leqq \text{NBOND} \leqq 5$. The negative integers denote that both ends of the bonds terminate at the ellipsoids. The positive integers denote bonds ending either at the ellipsoid or the tangent cone, as described previously in this section. An entry of zero draws no bond. A magnitude of 1 for NBOND produces two lines, one for each bond edge, 180° apart in the plane normal to the bond axis. Lines are drawn 90°, 45°, 22.5°, or 11.25° apart for NBOND magnitudes of 2, 3, 4, or 5, respectively. The back side of the bond is not drawn. Representative samples are shown in Fig. 6.1.

2. The bond radius (mean value for stick bonds) is in Angstrom units. Values between 0.01 and 0.06 A usually give good results. Any positive value may be used as long as it is smaller than the scaled ellipsoid minimum semidimension. The bond radius is not changed by the ellipsoid scale factor ratio SCAL2.

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[8]The accentuated taper may be increased or decreased by changing the value assigned to TAPER in SUBROUTINE PRIME (see TAPER in sect. 4.5).

3. The height of perspective labels for bond distances is entered as zero if no bond distances are to be labeled. Positive values denote the lettering height in inches before projection.

4. The perpendicular offset for bond distance perspective labels (in inches) pertains to offset of the center of the distance label relative to the center of the bond.

5. The height of regular labels for bond distances is entered as zero if no bond distances corresponding to foreshortened bonds are to be drawn. Positive values give the lettering height in inches before projection.

6. The perpendicular offset for bond-distance regular labels has the same definition as parameter 4 above.

7. The significant digits indicator is −1, 0, or 1, denoting bond distance labels with one, two, or three digits, respectively, after the decimal place.

Instructions 801, 802, and 803 differ from 811, 812, and 813 only in the monitor output listing. The second group has no output except error messages. The first group lists: (1) plotter coordinates in inches, (2) scaled Cartesian coordinates (in inches) of atom before projection, and (3) triclinic crystal coordinates for the atoms of each bond. The interatomic bond distance in angstroms is also listed. If an atom of a bonded pair is out of bounds, a fault message (NG = 10) is printed on the monitor output. If the bond is hidden and cannot be drawn, fault message NG = 14 is printed. Fault NG = 13 signifies that an imaginary intersection was found with a bond radius larger than the ellipsoid semidimension.

3.3.9.1 Instructions 801 and 811, Explicit Stick Bonds. – The only entry on the instruction card is the instruction number. A Format No. 2 trailer card is required with the fields specified under column 801 in Table 3.1 properly filled in. The bonds are described with two atom designator codes for each bond. The two atom designator codes for a bond must be in adjacent fields, but blank fields can be inserted between the different bonds. Since there are seven fields available per card, it is a good idea to use only two, four, or six of them so that the card sequence within the instruction (other than first and last cards) will be unimportant.

3.3.9.2 Instructions 802 and 812, Implicit Stick Bonds. – All parameters are input with Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the instruction number.

3.3.9.3 Instructions 803 and 813, Implicit Line Bonds. – All parameters are input with Format No. 2 trailer cards (see Table 3.1). The centered symbol placed on a given atom will be the centered symbol whose calling number corresponds to the atom number modulo 10 (see Fig. 4.2).

3.3.10 Label Plotting Instructions (900 Series). – The 900 series allows the user to plot general titles up to 72 characters in length, chemical symbols up to 6 characters long, bond length labels, and centered symbols. The bond length labels can have two decimal places before the decimal point and one, two, or three places after the decimal point. The 700 and 800 series instructions can plot chemical symbols and bond length labels, but it is often desirable to position certain labels individually with the 900 series.

General titles and bond length labels can be drawn either in perspective or parallel to the plane of the drawing. Chemical symbols and centered symbols are always drawn parallel to the plotter plane.

Instructions 913 through 916 are for perspective lettering, and instructions 901 through 909 produce regular lettering.

Two vectors, the upright vector and the base-line vector, are needed to describe a lettering plane. In OR TEP the upright lettering vector is always parallel to the plane of the drawing. For perspective lettering the base-line vector is a general vector in three dimensions. In the nonperspective case the base-line vector is either along the projection of a general vector or along the vector (in the plane of the plotter) which is oriented with 302 title rotation instruction (theta base line). If theta (set by 302) is zero, then the theta base-line vector is along the plotter positive x axis.

The exact center of the label is always referred to when specifying the position of the label. The program goes through the following steps to position the center point of the label onto the drawing. (1) A point $P1$ is found which is either the position of atom A or the mean of two atom positions (atom A and atom B). The atom A position is used if no atom designator exists in the atom B field of the instruction card. (2) A point $P2$ is found by (*a*) translating from $P1$ along the base-line vector for the distance specified by *parallel offset*, then (*b*) translating along the upright vector by the *perpendicular offset* distance. (3) A point $P3$ is found by projecting $P2$ onto the plane of the plotter. (4) If the x *edge reset* is >0, then x is reset to this value. If x *edge reset* is <0, x is reset to the positive x plot boundary minus $|x$ *edge reset*$|$. No resetting is done if x *edge reset* is zero. The y parameter is handled in the same manner with y *edge reset*.

The format for the entire 900 series is as follows:

Columns	
1–3	Blank or 3 (or 1 if second card is needed)
4–9	Instruction number
10–18	Designator for atom A
19–27	Designator for atom B (or blank)
28–36	x edge reset (in.)
37–45	y edge reset (in.)
46–54	Lettering height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
	Second Card (if needed)
1–3	Blank
4–9	Blank
10–18	Centered symbol number (0–14)

3.3.10.1 Instruction 901. – A nonperspective chemical symbol with theta base line is drawn using the chemical symbol for atom A.

3.3.10.2 Instruction 902. – A nonperspective title with theta base line is drawn. The title must be entered with the instructions on a Format No. 3 trailer card. The title should be centered about columns 36–37 of that card.

3.3.10.3 Instructions 903 and 913. – A general vector title is drawn with nonperspective lettering for 903 and perspective lettering for 913. The general vector is from atom A to atom B. The title is entered as described for 902 (see 3.3.10.2 above).

3.3.10.4. Instructions 904, 905, 906, 914, 915, and 916. – These are instructions for general-vector bond-length labels. The first three are for nonperspective lettering with one, two, and three places after the decimal point; and the last three are for the corresponding bond-length labels with perspective lettering. The general vector is from atom A to atom B. Note that the sense of the vector is important in order to have the label right side up.

3.3.10.5 Instructions 908 and 909. – These instructions are for centered symbols. With 908 the pen is up while moving to the position where the centered symbol is to be drawn, but *with 909 the pen is left down.* The centered symbol is one of the 15 listed for the CalComp SIMBOL routine (the misspelling of "symbol" is intentional). The symbol number must be in the range 0–14.

3.3.11 Saved Sequence Instructions (1100 Series). – It is often desirable to repeat a sequence of instructions one or more times with other instructions inserted between the repetitions. The 1100 series allows the user to do this without the necessity of putting in duplicate sequences of instruction cards. It is not an elaborate looping device, but it does give additional flexibility to the system.

The three instructions in this series are to start the saved sequence (instruction 1101), terminate the saved sequence (instruction 1102), and execute the saved sequence (instruction 1103). All instruction cards and their trailer cards between the 1101 and 1102 instructions are executed and saved on a magnetic scratch tape. A 1103 instruction rewinds this scratch tape and repeats all the instructions stored there before another instruction is read from the monitor input. There are no parameters to be entered with the 1100 series instructions.

3.3.12 Job Termination Instructions (Negative Series). – A (–1) instruction terminates the job and exits via SUBROUTINE EXIT.

A (–2) instruction reinitializes the whole program and starts over with another structure from the title card on. As many structures as desired may be run in sequence in this manner before exiting with a (–1) instruction. Note that the 201 instructions should occur only once and should not be repeated for succeeding jobs.

3.4 List of Fault Indicators

Certain errors are checked for in OR TEP, and when one of these occurs, an error message, "FAULT NG = *ng ADC m*" is written on the monitor output tape. The number NG is explained below. The *ADC* and *m* identify the atom code and the instruction involved (if these are relevant). If possible, corrective measures are made by OR TEP and the calculation proceeds; otherwise, the job is terminated by calling SUBROUTINE EXIT.

NG	Subroutine Involved	Fault	Action
1	PRELIM	No sentinel found after reading 48 symmetry cards	Tries to read parameter cards
2	PRELIM	No sentinel found after reading the parameter cards for 200 atoms	Tries to read instruction cards
3	PRELIM	Anisotropic temperature factor coefficients form a matrix which is not positive definite	EXIT after printing out all rms principal values (imaginary ones are negative)
4	ATOM,PAXES	Symmetry operation number is higher than the number of input operations	Omit atom
5	ATOM,PAXES	Atom number is higher than the number of input atoms	Omit atom
6	EIGEN	Null temperature factor matrix or failure in bisection routine	EXIT, after printing out all principal values
7	EIGEN	Eigenvector routine failure due to null vector	EXIT, after printing out all principal values
9	MAIN,SPARE	Unidentified instruction number	Omit faulty instruction
10	BOND,F700	Atom out of bounds	Omit atom
11	F800	No vector search codes	Omit instruction
12	F600	Insufficient number of atoms in ATOMS list	EXIT
13	BOND	Imaginary bond intersection	Omit bond
14	BOND	Hidden (end-on) bond	Omit bond
15	F900	Null vector as base line	Omit label

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

Certain of the numerical procedures[1] used in OR TEP are of a nature somewhat unfamiliar to many crystallographers. These aspects are outlined for the benefit of the reader who may wish to write a similar program or modify the present one.

4.1 Graphic-Computational Methods

These are the techniques used in producing the graphical details of the illustrations.

4.1.1 Drawing Ellipsoids. – Figure 3.1 demonstrates the various ellipsoid graphical representations that can be drawn with OR TEP. The major components in the representations are the three principal ellipses and the boundary (outline) ellipse. The principal ellipses have a front half and a back (hidden) half. The entire boundary ellipse is visible.

An ellipse is approximated by connecting a series of points on the ellipse with straight line segments. Points on an ellipse having a general orientation in three dimensions are computed; then each of these points is projected onto the drawing board for plotting.

The basic algorithm for finding the points along a given general ellipse utilizes the properties of conjugate diameters. Assume that we have the three principal axis vectors **V1**, **V2**, **V3** of the general ellipsoid and a vector **V4** from the center of the ellipsoid to the viewpoint. The vector **V5** normal to the polar plane (see Fig. 4.1), whose pole is the viewpoint, can be obtained from

$$\mathbf{V5} = \mathbf{A}\,\mathbf{V4}\ , \tag{4.1.1.1}$$

where **A** is the matrix for the ellipsoid which is defined by

$$\mathbf{X}^T\,\mathbf{A}\,\mathbf{X} = d\ , \tag{4.1.1.2}$$

where d is a constant.

The boundary ellipse is defined by two conjugate vectors, one of which is any vector **V6** perpendicular to **V5** and the second is **V7**, where

$$\mathbf{V7} = \mathbf{V5} \times \mathbf{A}\,\mathbf{V6}\ . \tag{4.1.1.3}$$

The assumption made for this boundary ellipse derivation is that the view distance is large compared to the ellipsoid size. Therefore, the boundary ellipse defined above always lies on the diametral polar plane (see Fig. 4.1).

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[1]For a treatment of the solid analytical geometry involved, the following three books are recommended. The first one is particularly useful.

J. Heading, *Matrix Theory for Physicists*, chap. 3, pp. 81–106, Longmans, Green and Co., London, 1958.

B. Spain, *Analytical Quadrics*, Pergamon Press, New York, 1960.

G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers*, McGraw-Hill Book Company, New York, 1961.

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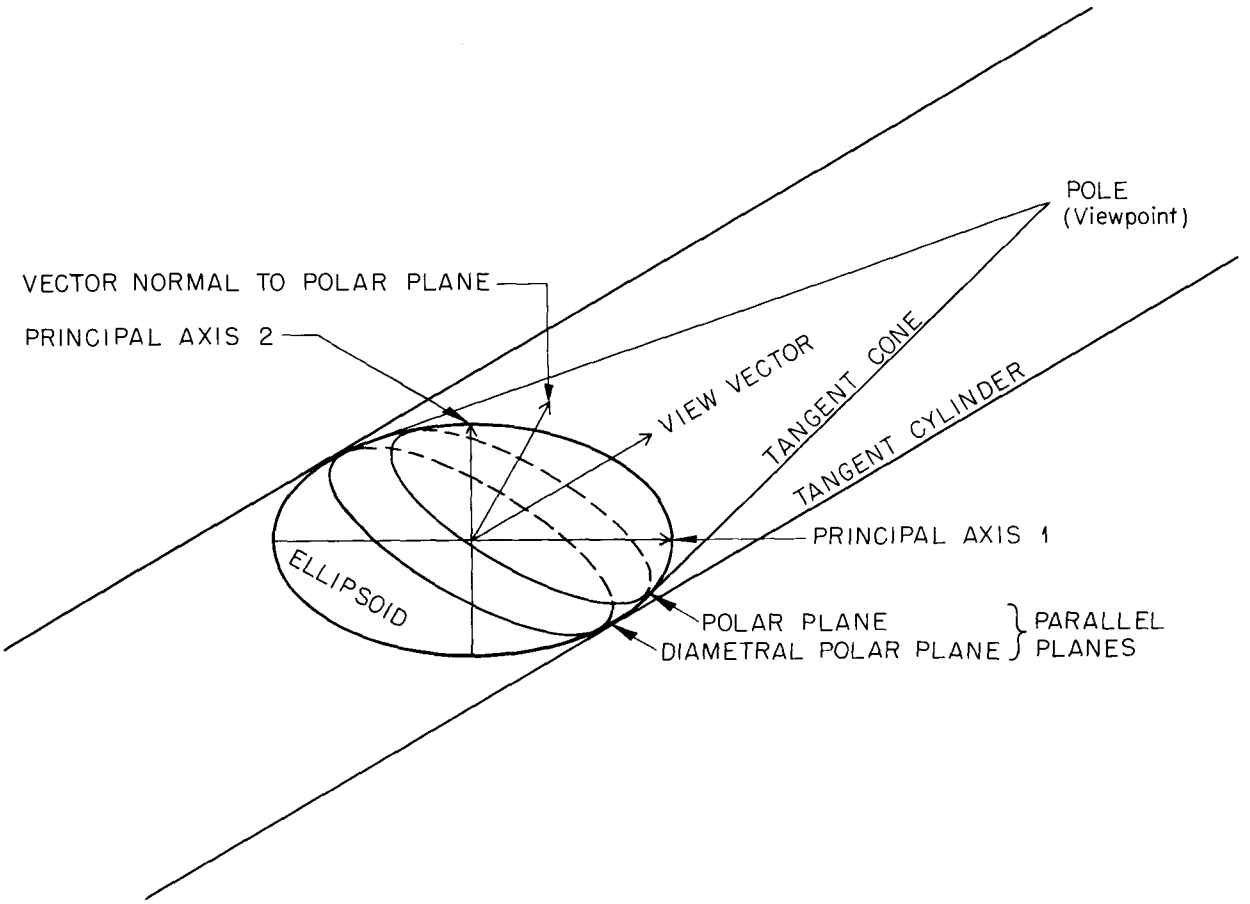

Fig. 4.1. Polar Planes Formed by Tangent Cylinder and Tangent Cone.

A principal ellipse which lies in the plane of the principal axis vectors **V1** and **V2** will have the third principal axis vector **V3** normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector **V8** where

$$\mathbf{V8} = \mathbf{V5} \times \mathbf{V3} \ . \tag{4.1.1.4}$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to **V8** and in the principal plane containing **V1** and **V2** is **V9**, where

$$\mathbf{V9} = \mathbf{V3} \times \mathbf{A}\,\mathbf{V8} \ . \tag{4.1.1.5}$$

After the conjugate vectors have been found, their lengths are adjusted to make them satisfy (4.1.1.2) by letting $\mathbf{X} = s\,\mathbf{l}$ where $\mathbf{l}$ is a unit vector. Solving for s, we obtain

$$s = [d/(\mathbf{l}^T\,\mathbf{A}\,\mathbf{l})]^{1/2} \ . \tag{4.1.1.6}$$

A conjugate vector pair is expanded into an ellipse by subroutine RADIAL. Since an ellipse is centrosymmetric, the two conjugate vectors and their negatives give us four vectors whose end points lie on the ellipse. By performing a vector sum of two adjacent vectors and dividing the resultant vector components by $\sqrt{2}$, we can obtain an additional vector. After doing this for all adjacent pairs, we then have a total of eight vectors. This process can be repeated as many times as desired except that the scaling constant will be different for each cycle. The constant is described by

$$\text{CONT}\,(i) = \{2[1 + \cos\,(\pi/i)]\}^{1/2}$$

where i is the cycle number.

This total process may be thought of as taking a planar radial set of equally spaced unit vectors and performing a deformation and scaling on the space in which it is described. In geometry this deformation is called an affine transformation.

Complete details on drawing ellipsoids can be obtained from the FORTRAN coding of subroutines F700 and RADIAL.

4.1.2 Drawing Bonds. – The major problem in drawing bonds is to obtain the intersection where the bond penetrates the ellipsoid. Three quadrics are used in subroutine BOND to calculate bond intersection. These three are the ellipsoid, the tangent cylinder, and the tangent cone.

The ellipsoid is described in matrix notation as

$$\mathbf{X}^T \mathbf{A}\, \mathbf{X} = d\,, \tag{4.1.2.1}$$

where d is a constant and $\mathbf{X}$ is any vector from the center to the surface of the ellipsoid. The matrix $\mathbf{A}$ is 3 by 3 symmetrical with components a_{ij} $(i,j = 1, 2, 3)$.

The elliptic cylinder tangent to the ellipsoid and with its axis along z is described by

$$\mathbf{X}^T \mathbf{B}\, \mathbf{X} = d\,, \tag{4.1.2.2}$$

where

$$\mathbf{B} = \begin{pmatrix} a_{11} - \dfrac{a_{13}a_{31}}{a_{33}} & a_{12} - \dfrac{a_{23}a_{31}}{a_{33}} & 0 \\ a_{12} - \dfrac{a_{13}a_{32}}{a_{33}} & a_{22} - \dfrac{a_{23}a_{32}}{a_{33}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.1.2.3}$$

and d is the constant used in (4.1.2.1). The tangent cylinder is used when it is necessary to terminate the bond at the boundary of the ellipsoid *when a parallel projection is used.*

To find the intersection of a cylindrical bond along $\mathbf{Vb}$ with radius r with either the ellipsoid or the tangent cylinder, we proceed as follows:

1. Form a radial set of vectors $\mathbf{Vr}_j$ of length r normal to $\mathbf{Vb}$.

2. Take a unit vector **l** parallel to **Vb** and let

$$\mathbf{X}_j = \mathbf{Vr}_j + s\,\mathbf{l}\,, \tag{4.1.2.4}$$

where s is a constant to be determined. Substituting in (4.1.2.1) we obtain

$$s^2 \mathbf{l}^T \mathbf{A}\,\mathbf{l} + 2s\,\mathbf{Vr}^T \mathbf{A}\,\mathbf{l} + \mathbf{Vr}^T \mathbf{A}\,\mathbf{Vr} - d = 0\,; \tag{4.1.2.5}$$

solving for s we get

$$s = \frac{-\mathbf{Vr}^T \mathbf{A}\,\mathbf{l} + \sqrt{(\mathbf{Vr}^T \mathbf{A}\,\mathbf{l})^2 - (\mathbf{l}^T \mathbf{A}\,\mathbf{l})(\mathbf{Vr}^T \mathbf{A}\,\mathbf{Vr} - d)}}{\mathbf{l}^T \mathbf{A}\,\mathbf{l}}\,. \tag{4.1.2.6}$$

The elliptic cone which is tangent to the ellipsoid and which has its apex on the viewpoint can be obtained from the matrix **A** and from the vector **Vu** which extends from the center of the ellipsoid to the viewpoint. This is performed in the following steps:

1. The ellipsoid is transformed with a rotation matrix to a new Cartesian frame of reference which has the z axis along the view vector **Vu**.
2. The tangent cone can now be described as

$$\mathbf{Y}^T \mathbf{C}\,\mathbf{Y} = 0\,, \tag{4.1.2.7}$$

where **Y** is a vector originating from the vertex (viewpoint) of the cone and

$$\mathbf{C} = \begin{pmatrix} a_{11} + \dfrac{a_{13}a_{31}}{K - a_{33}} & a_{12} + \dfrac{a_{13}a_{32}}{K - a_{33}} & \dfrac{Ka_{13}}{K - a_{33}} \\ a_{21} + \dfrac{a_{23}a_{31}}{K - a_{33}} & a_{22} + \dfrac{a_{23}a_{32}}{K - a_{33}} & \dfrac{Ka_{23}}{K - a_{33}} \\ \dfrac{Ka_{31}}{K - a_{33}} & \dfrac{Ka_{32}}{K - a_{33}} & \dfrac{Ka_{33}}{K - a_{33}} \end{pmatrix}, \quad K = d/|\mathbf{Vu}|\,. \tag{4.1.2.8}$$

3. The frame of reference is rotated back to its original orientation with a rotation matrix which is the inverse of the one used in step 1. Note that the origin is now on the viewpoint rather than the ellipsoid center.

To find the length, s, of a vector s **l** extending from any point p inside the cone to the surface of the cone we let

$$\mathbf{Y} = \mathbf{Vp} + s\,\mathbf{l} \tag{4.1.2.9}$$

and obtain from (4.1.2.7)

$$(\mathbf{Vp} + s\,\mathbf{l})^T\,\mathbf{C}\,(\mathbf{Vp} + s\,\mathbf{l}) = 0\,;$$

then solving for s we obtain

$$s = \frac{-\mathbf{V}\mathbf{p}^T \mathbf{C}\,\mathbf{l} + \sqrt{(\mathbf{V}\mathbf{p}^T \mathbf{C}\,\mathbf{l})^2 - (\mathbf{l}^T \mathbf{C}\,\mathbf{l})(\mathbf{V}\mathbf{p}^T \mathbf{C}\,\mathbf{V}\mathbf{p})}}{\mathbf{l}^T \mathbf{C}\,\mathbf{l}} . \tag{4.1.2.10}$$

The vector $\mathbf{V}\mathbf{p}$ from the vertex to $\mathbf{p}$ is formed by

$$\mathbf{V}\mathbf{p} = -\mathbf{V}\mathbf{u} + \mathbf{V}\mathbf{r} ,$$

where $\mathbf{V}\mathbf{r}$ is any member of a radial set such as that described for the regular ellipsoid intersection.

4.2 OR TEP Subprograms

The subprograms can be grouped into four functional categories. These can be called Mainstream, Subsidiaries, Arithmetic, and Plotting. The first three categories are coded in a FORTRAN dialect which will compile with either IBM-7090 FORTRAN II or CDC-1604A FORTRAN 63. The plotting routines are generally different for each machine configuration and are usually written in a machine-oriented symbolic language. In general, the standard library plotting routines available at most computing centers can be used with very minor modification.

4.2.1 Mainstream Subprograms. – The first three (PRIME, PRELIM, and MAIN) are the general controlling routines, and the remainder are oriented toward particular OR TEP instructions.

4.2.1.1 **PRIME.** – This routine "primes the program" by initializing all the "primer parameters" including the magnetic tape logical number assignments.

4.2.1.2 **PRELIM.** – All calculations concerned with processing (e.g., principal axis transformations) and storing the input crystallographic parameters are performed by PRELIM.

4.2.1.3 **MAIN.** – MAIN is the controlling routine which decodes the OR TEP instructions. It either executes the command directly or calls the appropriate subroutine which can execute the instruction.

4.2.1.4 **F200.** – This is the plotter "nursemaid routine" which is controlled through the 200 series instructions. It satisfies the whims and fancies of any particular plotting system control package.

4.2.1.5 **F400.** – This is the subroutine that executes the 401 and 411 instructions.

4.2.1.6 **F500.** – This is the subroutine that executes all 500 series instructions.

4.2.1.7 **F600.** – This is the subroutine that executes all 600 series instructions

4.2.1.8 **F700.** – This is the ellipsoid plotting routine, which executes all 700 series instructions.

4.2.1.9 **F800.** – This is the subroutine that executes all 800 series instructions. Bonds to be drawn are found by F800, then drawn by subroutine BOND.

4.2.1.10 **F900.** – This is the subroutine that executes all 900 series instructions.

4.2.1.11 **F1000.** – This is a dummy subroutine which is called by the presently nonexistent 1000 series instructions. This series can be coded by the user for any special purpose which may develop.

4.2.1.12 **SPARE(NJ).** – Further expansion of the instruction list may be done through this dummy subroutine, which is called by any $NJ \geqq 12$. NJ = instruction/100.

4.2.2 Subsidiary Subprograms. – 4.2.2.1 ATOM(ADC,X), DIMENSION X(3). – This will find the triclinic coordinates **X** for the atom described by the atom designator code ADC.

4.2.2.2 BOND (ADC1, ADC2, NB). – BOND is the bond plotting routine to draw a bond, described by Format No. 2 trailer card number NB, between atoms ADC1 and ADC2.

4.2.2.3 DRAW (W,DX,DY,NPEN), DIMENSION W(3). – DRAW interconnects OR TEP and the plot package. It also prevents the pen from crossing the boundaries. If the indicator ITILT in common is zero, the array W contains x and y in plotter coordinates. While perspective lettering is being plotted, ITILT $\neq 0$; and W contains x, y, z in Cartesian coordinates, which will be rotated and projected by DRAW to form plotter x,y coordinates. DX and DY are added to the plotter x and y, respectively, before the plot package is called. NPEN = 2 for pen down and 3 for pen up.

4.2.2.4 ERPNT (ADC,INST). – This is the printout routine called when a Fault is found. The arguments identify the atom designator code and the instruction involved in the Fault. The fault indicator, NG, is in common.

4.2.2.5 PAXES (ADC,ITYPE). – The covariance (dispersion) matrix for the thermal ellipsoid or its inverse matrix, which is the matrix of coefficients in the quadratic form describing the ellipsoid, is stored in common at Q for the atom ADC.

ITYPE > 0 for covariance matrix

ITYPE < 0 for ellipsoid quadratic form matrix

$|$ITYPE$| = 1$ based on triclinic system

$|$ITYPE$| = 2$ based on working Cartesian system

$|$ITYPE$| = 3$ based on reference Cartesian system

4.2.2.6 PLTXY (X,Y), DIMENSION X(3),Y(2). – This calculates the plotter coordinates Y from the unscaled Cartesian coordinates X. The distance to the closest boundary of the plot is placed in common at location EDGE.

4.2.2.7 PROJ (D,DP,X,XO,VIEW,I1,I2,I3), DIMENSION D(3,129),DP(2,129),X(3),XO(3). – This routine is used to obtain an array, DP, of plotter coordinates from a scaled array, D, of points described in Cartesian coordinates. X, XO, and VIEW are parameters involved in the projection, and I1, I2, I3 are DO loop parameters for indexing through the array.

4.2.2.8 RADIAL(ND). – Given two conjugate radius vectors of an ellipse in the array DA in common, RADIAL generates a "radial" array (D in common) of points lying on the ellipse. From 8 to 128 points are generated depending on the value of ND ($1 \leqq$ ND $\leqq 5$).

4.2.2.9 SEARCH. – Instructions 101, 102, 402, and 403 utilize this routine to conduct an exhaustive (but educated) search to find all points within a sphere or rectangular box. Interatomic distances and angles are also calculated for the 100 series.

4.2.2.10 STORE. – This routine stores atoms in (or removes atoms from) the ATOMS array. Coordinates in whichever system is in use and the atom designator code are communicated to STORE via array V1 of common.

4.2.2.11 XYZ(ADC,X,ITYPE), DIMENSION X(3). – Coordinates for atom ADC are returned in X.

ITYPE = 0: triclinic coordinates

ITYPE = 1 or 2: working Cartesian system coordinates

ITYPE = 3: reference Cartesian system coordinates

4.2.3 Arithmetic Subprograms. — 4.2.3.1 Function ARCCOS (X). — This routine computes θ, the arc cosine of X in degrees; $0 \leqq \theta \leqq 180°$.

4.2.3.2 AXEQB (A,X,B,N), DIMENSION A(3,3),X(3,3),B(3,3). — This routine solves the matrix equation **A X** = **B** for **X**. The matrices **B** and **X** are (3,N) and **A** is always (3,3). To invert **A**, make **B** an identity matrix.

4.2.3.3 AXES (X, Y, A, ITYPE), DIMENSION X(3),Y(3),A(3,3). — This routine provides three orthogonal column vectors in **A**, each 1 A long, from the two vectors **X** and **Y**.

ITYPE > 0: Cartesian system

ITYPE ≦ 0: triclinic system

|ITYPE| = 1: $\mathbf{A}_1 = \mathbf{X}$; $\mathbf{A}_2 = (\mathbf{X} \times \mathbf{Y})$; $\mathbf{A}_3 = \mathbf{X} \times (\mathbf{X} \times \mathbf{Y})$

|ITYPE| = 2: $\mathbf{A}_1 = \mathbf{X}$; $\mathbf{A}_2 = (\mathbf{X} \times \mathbf{Y}) \times \mathbf{X}$; $\mathbf{A}_3 = \mathbf{X} \times \mathbf{Y}$

ITYPE = 0: same as type 2 except **X** = *a* crystal axis, **Y** = *b* crystal axis.

4.2.3.4 DIFV (X,Y,Z), DIMENSION X(3),Y(3),Z(3). — This routine performs the vector subtraction **X** − **Y** = **Z**. **Z** may have the same location as **X** or **Y**.

4.2.3.5 EIGEN (A,X,B), DIMENSION A(3,3),X(3),B(3,3). — EIGEN determines the three eigenvalues **X** and the three column eigenvectors **B** of the matrix **A**. Indeterminate eigenvectors are replaced by zeros and the Fault indicator NG set to a negative value (eigenvectors are assigned for the indeterminate cases by PRELIM).

4.2.3.6 MM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3). — MM performs the matrix multiplication **A B** = **C**. The location of **C** must be different from **A** and **B**.

4.2.3.7 MV (A,X,Y), DIMENSION A(3,3),X(3),Y(3). — MV performs the matrix-vector multiplication **A X** = **Y**. The location of **Y** must be different from **A** and **X**.

4.2.3.8 NORM (X,Y,Z,ITYPE), DIMENSION X(3),Y(3),Z(3). — NORM stores at **Z** a vector (not necessarily a unit vector) perpendicular to both **X** and **Y**. The sense of **Z** is that of the vector product **X** × **Y**.

ITYPE > 0: Cartesian system

ITYPE ≦ 0: triclinic system

4.2.3.9 TMM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3). — TMM performs the matrix multiplication $(\mathbf{A}^T\ \mathbf{B})^T = \mathbf{C}$. The location of **C** must be different from **A** and **B**.

4.2.3.10 UNIT (X,Y,ITYPE), DIMENSION X(3),Y(3). — The vector **Y** is made 1 A long and parallel to **X**. The vectors **X** and **Y** may have the same location.

ITYPE > 0: Cartesian system

ITYPE < 0: triclinic system

4.2.3.11 VM (X,A,Y), DIMENSION X(3),A(3,3),Y(3). — VM performs the vector-matrix multiplication $\mathbf{X}^T\mathbf{A} = \mathbf{Y}^T$. The location of **Y** must be different from **X** and **A**.

4.2.3.12 FUNCTION VMV (X,A,Y), DIMENSION X(3),A(3,3),Y(3). — VMV performs the vector-matrix-vector multiplication $\mathbf{X}^T\mathbf{A}\ \mathbf{Y}$ = scalar.

4.2.3.13 FUNCTION VV (X,Y), DIMENSION X(3),Y(3). – VV performs the vector-vector multiplication $\mathbf{X}^T\mathbf{Y}$ = scalar.

4.2.4 Plotting Subprograms for the CalComp Plotter. – The plotting subroutines are taken from the Library routines currently in use at Oak Ridge National Laboratory with the CDC 1604A and the IBM 7090 computers. A CalComp model 580 Magnetic Tape Plotting System is used. The three major routines required are derived from the CalComp subroutines PLOTS, SYMBOL, and NUMBER. The OR TEP modifications are called PLOTS, SIMBOL, and NOMBER.

4.2.4.1 Subroutine PLOTS. – This is an unmodified CalComp Library routine with two entry points.

a) ENTRY – PLOTS (A, LENGTH, LTNO)

This is the initialization entry for the plotter package and should be used only once in the program. This call must be made prior to usage of any other subroutines in the package.

A is an array which may be used by the plotting package for storing data to be written on the plot tape.

LENGTH is the number of locations in A available to the plotter package.

LTNO is an integer which tells the plotter package the logical tape number of the plotter tape.

In subroutine F200 we have

DIMENSION PLA(2000)

and card F2000170 contains

"210 CALL PLOTS (PLA,2000, LTNO)"

for the CDC 1604A or

"210 CALL PLOTS (PLA(2000),1998,LTNO)"

for the IBM 7090. The reverse storage of common in the IBM 7090 is the reason for the difference. LTNO is in common and was set to 23 by subroutine PRIME.

An ORTEP 201 instruction directs the execution of this initialization.

b) ENTRY – PLOT (X,Y,IPEN)

This is the basic entry to convey data to the subroutine for plotting. To facilitate the substitution of other plotting routines, ORTEP contains only one instruction (card DRAW0320 in subroutine DRAW) which calls this entry point. All the plotting information passes through DRAW before going to the actual plotting routine PLOT.

X is the abscissa expressed in inches.

Y is the ordinate expressed in inches.

IPEN = 3, the pen will be lifted prior to execution of the movement to the given (**X**,**Y**) position.

IPEN = 2, the pen will be lowered to the paper and a straight line will be drawn from the current (**X**,**Y**) to the given (**X**,**Y**) position.

IPEN = –3, the subroutine will interpret this as being the end of the current plot; and, following movement to the new (**X**,**Y**) position, it will set **X** = 0.0, so that a new origin is established for the following plot (an ORTEP 202 instruction executes this termination procedure).

This subroutine keeps track of current **X** and **Y** positions, and whether or not the pen is in contact with the paper. It stores data in the array A provided by the programmer and writes out a record on the specified tape each time the storage area is filled or an end-of-plot call is made. It also generates sequential plot addresses for each plot on the magnetic tape, so that physical plotting of the plots can be done in any order, regardless of the order in which they were placed on tape.

4.2.4.2 Subroutine SIMBOL. – SIMBOL differs from the standard routine SYMBOL in two respects:

1. The input positional parameters specified in the input argument should be an array containing *X, Y, and Z* in adjacent memory locations. Three-dimensional parameters are required to produce perspective labels. The *Z* parameter is not used by SIMBOL but is transferred to another array that is referenced when SIMBOL calls DRAW.

2. The standard routine SYMBOL calls PLOT directly while SIMBOL calls DRAW which in turn calls PLOT. When perspective labels are used, DRAW will perform a three-dimensional rotation and a projection of the grid points on which the letters are formed, to obtain true perspective. The calling sequence for DRAW is described in 4.2.2.3.

There are two uses of subroutine SIMBOL. The first use is for producing labels, and the second is for plotting one of 15 special centered symbols.

1. ENTRY – SIMBOL (X(1),X(2),H,BCD,THETA,N), DIMENSION X(3) (note $N \geqq 0$)

   X(1),X(2) are the *X* and *Y* coordinates of the lower left-hand edge of the first character to be drawn.

   X(3) is the *Z* coordinate. It is used only with perspective labeling.

   H is the height in inches of the character to be drawn. The width of the character is equal to $^4/_7$ the height and the character spacing is $^6/_7$ the height.

   BCD specifies the address of an array containing the BCD characters to be plotted.

   THETA is the angle in degrees by which the base line of the characters is to be rotated counterclockwise from the positive *X* axis.

   N is an integer which specifies the number of characters in the array BCD that are to be drawn.

2. ENTRY – SIMBOL (X(1),X(2),H,NUM,THETA,L), DIMENSION X(3) (note $L < 0$)

   X(1),X(2) are the *X* and *Y* coordinates of the center of the symbol.

   H is the height of the symbol to be plotted.

   NUM is an integer such that $0 \leqq NUM \leqq 14$ which determines which symbol is to be plotted. A list of the integers and the symbols generated is shown in Fig. 4.2.

   THETA is the angle of rotation as described previously.

   $L = -1$: the centered symbol will be plotted without a line being drawn from the previous (X,Y) position.

   $L < -1$: a straight line will be drawn from the previous (X,Y) position to the given (X,Y) position.

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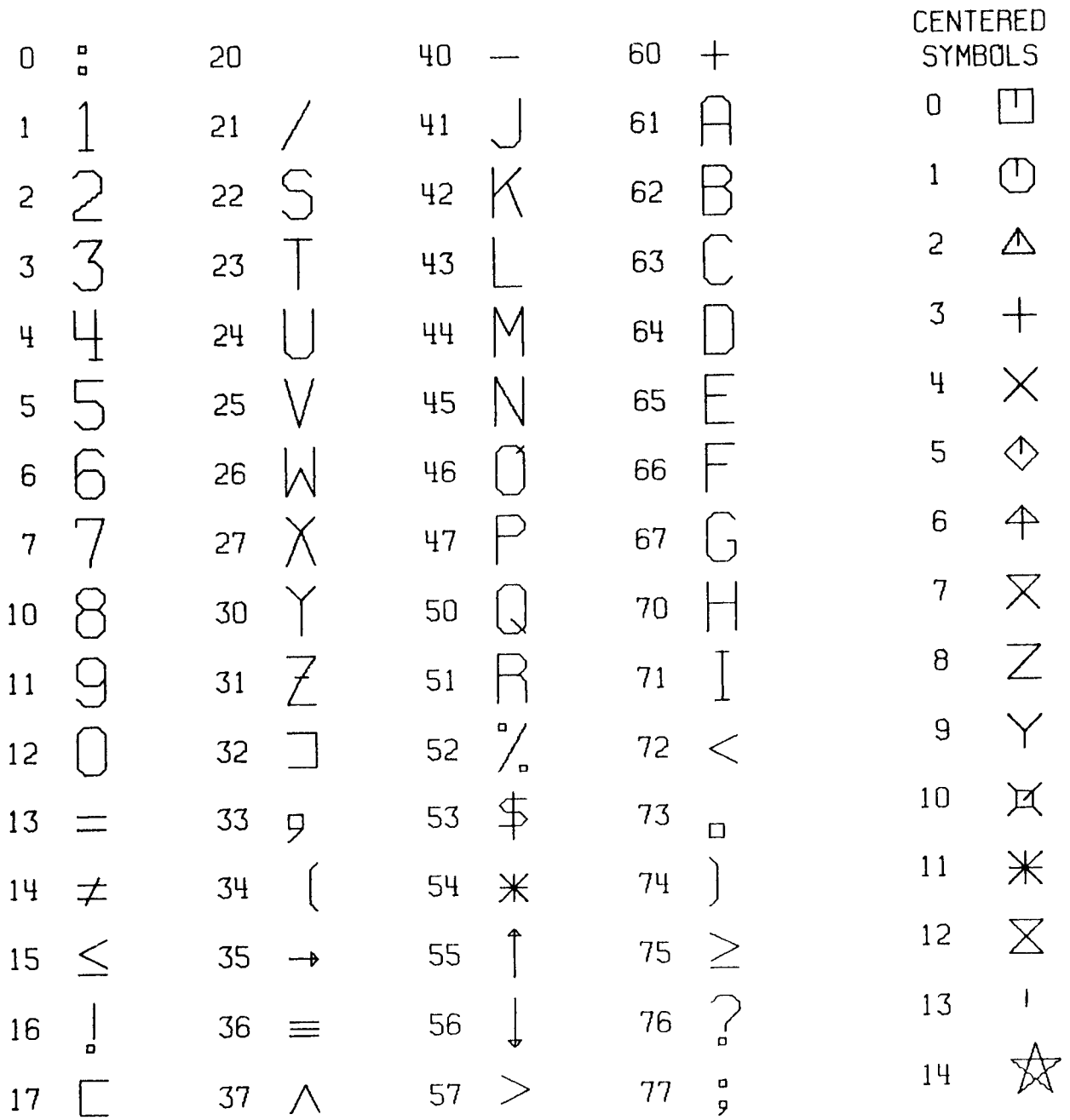

Fig. 4.2. Characters Available in 1604-A Symbol Routine.

4.2.4.3 Subroutine NOMBER. – This is a subroutine to convert a machine format number to its BCD equivalent and plot it according to a specified format.

NOMBER is different from the usual subroutine NUMBER in that it calls SIMBOL rather than SYMBOL.

ENTRY – NOMBER(X(1),X(2),H,A,THETA,nHFORMAT)

X(1),X(2),H and THETA are described in Sect. 1 of the SIMBOL routine.

A is the address of the floating or fixed point number which is to be plotted.

nHFORMAT is a BCD argument which specifies the manner in which the number is to be converted and plotted.

4.3 Adapting OR TEP to Other Equipment Configurations

Card decks[2] for ORTEP will be provided free of charge to crystallographers and others who request that the deck be sent to them.

The card deck contains:

1. The FORTRAN source deck with all FORTRAN subprograms arranged alphabetically. An exception is MAIN, which is first in the deck. The deck is set up for compilation by IBM 7090 FORTRAN II. The changes required to compile the deck with CDC 1604 FORTRAN 63 are described in 4.3.1.
2. Either the FAP plotting subroutines for use on the IBM 7090 or the CODAP plotting subroutines for the CDC 1604 will be sent if so requested by the user.
3. Complete binary deck for either the IBM 7090 or the CDC 1604A.
4. Cards for the example figure, cubane.

4.3.1 OR TEP Source Deck Differences for the IBM 7090 and the CDC 1604A. – The following changes should be made to set up the FORTRAN source deck for compilation with CDC 1604 FORTRAN 63.

1. Remove the "*LIST8" and "*LABEL" cards which precede each subprogram.
2. Place a "PROGRAM MAIN" card just before card MAIN0010.
3. Replace card F2000170 with "210 CALL PLOTS (PLA,2000,LTNO)."
4. Replace PRIM0210 with IN = 50,
   PRIM0270 with NOUT = 51,
   PRIM0280 with NSR = 57,

or with whatever numbers the monitor system requires for Input, Output, and Scratch tapes.

The coding of the plotting routines is completely different for the two systems. In addition, the IBM 7090 plot package contains two subroutines, TRW2 and MSG, which the CDC 1604 package does not have.

[2]The size of the card deck (3000–5000 cards) is such that it is generally more economical to send the program on magnetic tape. If convenient, the user should send a blank magnetic tape to the author. Card images will be written on that tape in either 200 or 556 bit-per-inch density binary-coded-decimal and the tape returned to the sender. Alternately, the card deck will be sent if desired.

4.3.2 Magnetic Tape Logical Number Assignments. – Logical tape number assignments are made in subroutine PRIME. Four cards are involved in this initialization:

Magnetic Tape Function	Symbolic Name		Primer Constant	Location in PRIME
a) Monitor Input	IN	=	10	PRIM0210
b) Monitor Output	NOUT	=	9	PRIM0270
c) Scratch	NSR	=	11	PRIM0280
d) Plotting	LTNO	=	23	PRIM0240

4.3.3 Plotter Systems Other than the CalComp 580. – In general, only subroutine PLOTS (with entries PLOTS and PLOT) needs to be replaced when a different plotting system is used. This routine is called from only two locations, one in F200 and the other in DRAW. F200 will probably have to be rewritten, and the 200 series instructions may have to be redefined and expanded to accommodate the rules of the new system.

Location DRAW0320 in subroutine DRAW should also be modified to call the new line-drawing routine with the correct argument.

4.3.4 Computing Systems Other than the CDC 1604A and IBM 7090. – Basically, the OR TEP system is designed to be used in a 32 K memory. There are about 7000_{10} unused cells when the system operates with a 32 K word IBM 7090. Consequently, OR TEP would have to be changed considerably to operate in a much smaller memory.

It is hoped that the FORTRAN subprograms will also compile on other machines, but this possibility has not been checked.

If it becomes necessary to replace the machine language subroutines SIMBOL and NOMBER with completely different routines, the statements calling these routines will also need to be modified.

SIMBOL is called from BOND0450, BOND0470, F7000080, F9001280, F9001310, and F9001450.

NOMBER is called from BOND2460, BOND2480, BOND2500, F9001380, F9001400, and F9001420.

4.4 Addition of New OR TEP Instructions

Occasions will arise when additional special purpose instructions would be useful. For example, perhaps a cell outline routine would be desirable. (Originally, the 1000 series of instructions were planned for drawing a parallelepiped defined by four general vectors. However, this feature later seemed somewhat redundant and was omitted, since crystal cell outlines can be produced with judicious usage of small dummy atoms and the 800 series instructions.)

The subroutines F1000 and SPARE are intended to be used for additional instructions. All 1000 series instructions call subroutine F1000, which is currently just a dummy routine. Instructions $\geqq 1200$ call another dummy routine, subroutine SPARE(NJ), where NJ = instruction number/100.

All Arithmetic subprograms (see 4.2.3) and many of the subsidiary subprograms (see 4.2.2) are available for coding these Mainstream subprograms (see 4.2.1).

4.5 Glossary of Symbols in OR TEP Common, with Array Dimensions

	A(9)	Direct crystal cell parameters, a, b, c, cos α, cos β, cos γ, $\alpha(°)$, $\beta(°)$, $\gamma(°)$.
	AA(3,3)	Metric tensor **g** where $\mathbf{g}_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.
	AAREV(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the reference Cartesian system. **AAREV** = **AA REFV**.
	AAWRK(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the working Cartesian system. **AAWRK** = **AA WRKV**.
	AID(3,3)	Identity matrix.
	AIN(140)	Array containing the input parameters of the current OR TEP instruction.
	ATOMS(4,500)	Column 1 contains atom designator codes for the atoms which are to be included in the scaling, plotting, bond searching, etc. The other three columns are used for temporary storage of coordinates in any of several coordinate systems.
	BB(3,3)	Reciprocal metric tensor. **BB** = $\mathbf{AA}^{-1}$.
P	BRDR	Border width in inches extending inward from plot boundary.
	CD(8,20)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(200)	Chemical symbols for the input atoms.
P	CONT(5)	Constants used in subroutine RADIAL.
	D(3,130)	Array in which three-dimensional points on an ellipse are stored by RADIAL.
	DA(3,3)	Transmits conjugate vectors to RADIAL. Also used for temporary storage.
	DP(2,130)	Array in which two-dimensional points for ellipse are stored after projection.
P	DISP	Displacement parameter for retracing.
	EDGE	Distance in inches from a projected point to the closest boundary. Set in PLTXY.
	EV(3,200)	Root-mean-square displacements for each principal axis of each input atom.
P	FORE	Cosine of critical angle between bond and Cartesian z axis vectors for perspective bond distance labels. At smaller angles the labels, produced from subroutine BOND, are drawn without perspective to prevent excessive foreshortening.
	FS(3,3,48)	Rotation matrices for input symmetry operations based on triclinic system. Used with TS array.
P	IN	Logical number for monitor input magnetic tape.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling ("Tilted Titles").
	KD(5,20)	Part of vector search code array. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
P	LTNO	Logical tape number for magnetic plotting tape.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction (vector search codes).

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	NG	FAULT INDICATOR (see 3.4).
	NJ	Instruction number/100.
	NJ2	Last two decimal digits of the instruction number (instruction = NJ*100 + NJ2).
P	NOUT	Logical number for monitor output magnetic tape.
P	NSR	Logical number for scratch magnetic tape.
	NSYM	Number of input symmetry operations.
	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).
	P(3,200)	Triclinic positional coordinates for the input atoms.
	PA(3,3,200)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 A long, based on the triclinic system (principal axis vectors).
	PAC(3,5)	A 3 × 3 matrix produced by subroutine PAXES and made up of three orthonormal principal axis column vectors, based on either the working or reference Cartesian system. Columns 4 and 5 are used in subroutine F700 to duplicate columns 1 and 2 for ease in indexing.
	PAT(3,3)	A matrix produced by subroutine PAXES and composed of three principal axis column vectors each 1 A long, based on the triclinic system.
	Q(3,3)	A matrix produced by subroutine PAXES. Contains either the dispersion matrix or its inverse, based on either the working or reference Cartesian systems.
	REFV(3,3)	A matrix made up of three orthogonal column vectors, each 1 A long, based on the triclinic system. This is the base vector triplet for the reference Cartesian coordinate system. The transpose is the postfactor transformation matrix for converting coordinates from the reference orthogonal system to the triclinic system. $\mathbf{REFV}^T = \mathbf{AAREV}^{-1}$.
P	RES(4)	Regulates the resolution of the plotting of a given ellipse as a function of the longest principal axis x in the given ellipsoid of the scaled model.

$x \geqq$ Res(1)	128-point ellipse
Res(1) $> x \geqq$ Res(2)	64-point ellipse
Res(2) $> x \geqq$ Res(3)	32-point ellipse
Res(3) $> x$	16-point ellipse
Res(4) is not used.	

	RMS(5)	The rms displacements along the principal axes in arrays PAC and PAT.
P	SCAL1	The scale of the model in inches per angstrom before projection.
P	SCAL2	The scale factor ratio which sets the ellipsoid scale relative to SCAL1. If SCAL2 = 1.54, then the instantaneous position of the atomic center will be within the ellipsoid 50% of the time (50% probability ellipsoid).
P	SCL	SCL = SCAL1 times SCAL2.
P	SYMB(3,3)	A rotation matrix based on the angle THETA which is set by instruction 302.
P	TAPER	The exaggerated bond taper parameter. The top and bottom ends of a bond have radii: RADIUS = 1. ± TAPER *T6 where T6 = |cosine of angle between bond and z axis of Cartesian system| .

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	THETA	Angle in degrees between plotter x axis and lettering base-line vector.
	TITLE(12)	Alphanumeric job title storage.
	TITLE2(12)	Alphanumeric information storage for Format No. 3 trailer card.
	TS(3,48)	Translation vector for each input symmetry operation. Used with FS array.
P	VIEW	Viewing distance in inches.
	VT(3,4)	Perspective title rotation matrix and translation vector. Also used for temporary storage.
	V1(4)	Array to transfer data to subroutine STORE. Also used for temporary storage.
	V2(3) , ... , V6(3)	Temporary storage.
	WRKV(3,3)	Same definition as for REFV except that this one is for working Cartesian system. $\mathbf{WRKV}^T = \mathbf{AAWRK}^{-1}$.
P	XLNG(3)	Elements (1) and (2) are x and y plot dimensions. Element (3) is not used.
P	XO(3)	Elements (1) and (2) denote the position in plotter coordinates (in inches) where ORGN is placed. Element (3) is not used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS

It is convenient to develop the physical significance of the anisotropic temperature factor with the notation and terminology of probability theory rather than with the more familiar Fourier transform theory. The results are, of course, identical regardless of the terminology used. The reason for this choice is that the literature of mathematical statistics and probability theory is somewhat neater and easier to follow. The texts by Wilks,[1] Cramer,[2] Miller,[3] Hamilton,[4] and Lukacs and Lana[5] and the handbooks by Burington and May[6] and Owen[7] are found to be particularly useful.

5.1 Probability Density Function (pdf) of a Trivariate Normal Distribution

Given three chance variables X_1, X_2, X_3 and S which is a region in X_1, X_2, X_3 space. The probability $P(S)$ that the point (X_1, X_2, X_3) falls in the region S is given by

$$P(S) = \iiint_S \phi(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 \,. \tag{5.1.1}$$

If the integration is carried over all space, then

$$\iiint_{-\infty}^{\infty} \phi(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 = 1 \,. \tag{5.1.2}$$

The function $\phi(X_1, X_2, X_3)$ is called the probability density function (pdf) for the joint distribution of X_1, X_2, X_3. Using vector notation, we can designate the pdf as $\phi(\mathbf{X})$.

When the distribution is the type said to be normal or Gaussian, the pdf is

$$\phi(\mathbf{X}) = \frac{[\det(\mathbf{M}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp\left[-\tfrac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1} (\mathbf{X} - \hat{\mathbf{X}})\right] . \tag{5.1.3}$$

The matrix $\mathbf{M}^{-1}$ is the inverse of the symmetrical dispersion (variance-covariance) matrix $\mathbf{M}$, where

$$\mathbf{M} = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13} \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \sigma_2\sigma_3\rho_{23} \\ \sigma_1\sigma_3\rho_{13} & \sigma_2\sigma_3\rho_{23} & \sigma_3^2 \end{pmatrix} .$$

The symbols σ_i^2 represent the second moments or variances about the mean position $\hat{\mathbf{X}}$. The symbols $\sigma_i\sigma_j\rho_{ij}$ are the corresponding covariances and ρ_{ij} are the correlation coefficients.

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[1] S. S. Wilks, *Mathematical Statistics*, Wiley, New York, 1962.

[2] H. Cramer, *Random Variables and Probability Distributions*, Cambridge University Press, London, 1962.

[3] K. S. Miller, *Multidimensional Gaussian Distributions*, Wiley, New York, 1964.

[4] W. C. Hamilton, *Statistics in Physical Science*, Ronald, New York, 1964.

[5] E. Lukacs and R. G. Lana, *Applications of Characteristic Functions*, Hafner Publishing Co., New York, 1964.

[6] R. S. Burington and D. C. May, *Handbook of Probability and Statistics with Tables*, Handbook Publishers, Sandusky, Ohio, 1953.

[7] D. B. Owen, *Handbook of Statistical Tables*, Addison-Wesley, Reading, Mass., 1962.

5.2 Equiprobability Ellipsoids

For a proper normal distribution the quadratic form $(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1} (\mathbf{X} - \hat{\mathbf{X}})$ is positive definite, and a principal axis transformation is possible which will make the cross correlation coefficients $\rho_{ij} = 0$ $(i \neq j)$. This transformation is discussed in 5.4. The result of the transformation is the pdf

$$\phi(y_1, y_2, y_3) = \frac{1}{(2\pi)^{3/2} \sigma_{y_1} \sigma_{y_2} \sigma_{y_3}} e^{-Q/2} , \tag{5.2.1}$$

where

$$Q = \frac{(y_1 - \hat{y}_1)^2}{\sigma_{y_1}^2} + \frac{(y_2 - \hat{y}_2)^2}{\sigma_{y_2}^2} + \frac{(y_3 - \hat{y}_3)^2}{\sigma_{y_3}^2} . \tag{5.2.2}$$

The y_i are coordinates based on the Cartesian principal axis system and $\sigma_{y_i}^2$ are the variances along the principal axes, $i = 1, 2, 3$.

The normal probability density function is constant for points on the ellipsoid $Q = C^2$ where C is a constant. The probability that a random point (y_1, y_2, y_3) in the distribution will fall inside the ellipsoid is

$$P(C) = (2/\pi)^{1/2} \int_0^C r^2 e^{-r^2/2} \, dr . \tag{5.2.3}$$

This result is derived from (5.1.1), (5.2.1), and (5.2.2) by transforming to spherical coordinates.

When $C = 1.5382$, $P = 0.5$ and the corresponding ellipsoid is called the 50% probability ellipsoid. A table of P vs C values is found on page 203 of Owen's *Handbook of Statistical Tables.*[7] For convenience, that table is reproduced here as Table 5.1.

5.3 Characteristic Function (c.f.) of a Trivariate Normal Distribution

The characteristic function $\Phi(\mathbf{T})$ corresponding to a trivariate distribution $\phi(\mathbf{X})$ is the expected value of $e^{i\mathbf{T}^T\mathbf{X}}$, namely,

$$\Phi(\mathbf{T}) = \int_{-\infty}^{\infty} \phi(\mathbf{X}) e^{i\mathbf{T}^T\mathbf{X}} \, d\mathbf{X} . \tag{5.3.1}$$

For the trivariate normal pdf (5.1.3) the corresponding characteristic function is

$$\Phi(\mathbf{T}) = \exp\left[i\mathbf{T}^T\hat{\mathbf{X}} - \tfrac{1}{2}\mathbf{T}^T\mathbf{M}\mathbf{T}\right] , \tag{5.3.2}$$

where $\mathbf{M}$ is the variance-covariance dispersion matrix described in 5.1 and $\hat{\mathbf{X}}$ is the center of mass of the distribution.

The crystallographic structure factor equation which incorporates general anisotropic temperature factor coefficients is

$$F(\mathbf{h}) = \sum_n f_n(\mathbf{h}) \exp(2\pi i \mathbf{h}^T\hat{\mathbf{X}}_n) \exp(-\mathbf{h}^T\mathbf{B}_n\mathbf{h}) , \tag{5.3.3}$$

Table 5.1. Critical Values for Probability Ellipsoids of a Trivariate Normal Distribution[a]

P	C	P	C	P	C
0.01	0.3389	0.41	1.3842	0.81	2.1824
0.02	0.4299	0.42	1.4013	0.82	2.2114
0.03	0.4951	0.43	1.4183	0.83	2.2416
0.04	0.5479	0.44	1.4354	0.84	2.2730
0.05	0.5932	0.45	1.4524	0.85	2.3059
0.06	0.6334	0.46	1.4695	0.86	2.3404
0.07	0.6699	0.47	1.4866	0.87	2.3767
0.08	0.7035	0.48	1.5037	0.88	2.4153
0.09	0.7349	0.49	1.5209	0.89	2.4563
0.10	0.7644	0.50	1.5382	0.90	2.5003
0.11	0.7924	0.51	1.5555	0.91	2.5478
0.12	0.8192	0.52	1.5729	0.92	2.5997
0.13	0.8447	0.53	1.5904	0.93	2.6571
0.14	0.8694	0.54	1.6080	0.94	2.7216
0.15	0.8932	0.55	1.6257	0.95	2.7955
0.16	0.9162	0.56	1.6436	0.96	2.8829
0.17	0.9386	0.57	1.6616	0.97	2.9912
0.18	0.9605	0.58	1.6797	0.98	3.1365
0.19	0.9818	0.59	1.6980	0.99	3.3682
0.20	1.0026	0.60	1.7164	0.991	3.4019
0.21	1.0230	0.61	1.7351	0.992	3.4390
0.22	1.0430	0.62	1.7540	0.993	3.4806
0.23	1.0627	0.63	1.7730	0.994	3.5280
0.24	1.0821	0.64	1.7924	0.995	3.5830
0.25	1.1012	0.65	1.8119	0.996	3.6492
0.26	1.1200	0.66	1.8318	0.997	3.7325
0.27	1.1386	0.67	1.8519	0.998	3.8465
0.28	1.1570	0.68	1.8724	0.999	4.0331
0.29	1.1751	0.69	1.8932	0.9991	4.0607
0.30	1.1932	0.70	1.9144	0.9992	4.0912
0.31	1.2110	0.71	1.9360	0.9993	4.1256
0.32	1.2288	0.72	1.9580	0.9994	4.1648
0.33	1.2464	0.73	1.9804	0.9995	4.2107
0.34	1.2638	0.74	2.0034	0.9996	4.2661
0.35	1.2812	0.75	2.0269	0.9997	4.3365
0.36	1.2985	0.76	2.0510	0.9998	4.4335
0.37	1.3158	0.77	2.0757	0.9999	4.5943
0.38	1.3330	0.78	2.1012	0.99999	5.0894
0.39	1.3501	0.79	2.1274	0.999999	5.5376
0.40	1.3672	0.80	2.1544	0.9999999	5.9503

[a]Reproduced from Ref. 7 by permission of Addison-Wesley Publishing Company, Inc., Reading, Mass. The original caption was "Critical Values for the Spherical Normal Distribution."

where

$\mathbf{h}$ is a vector giving the Miller indices,

$\mathbf{X}_n$ is a vector giving the fractional unit cell coordinates of the nth atom,

$\mathbf{B}_n$ is the anisotropic temperature factor coefficient matrix, and

$f_n(\mathbf{h})$ is the atom form factor value for atom n.

If a change of variables $\mathbf{T} = 2\pi\mathbf{h}$ is made, then (5.3.3) can be rewritten as

$$F(\mathbf{T}) = \sum_n f_n(T) \exp\left(i\,\mathbf{T}^T\hat{\mathbf{X}}_n - \tfrac{1}{2}\,\mathbf{T}^T \frac{\mathbf{B}_n}{2\pi^2}\mathbf{T} \right) . \tag{5.3.4}$$

The scaled anisotropic temperature factor matrix $(1/2\pi^2)\mathbf{B}$ is seen to be identical with the variance-covariance dispersion matrix $\mathbf{M}$ in (5.3.2).

The corresponding crystal space trivariate normal pdf for any particular atom n is

$$\phi(\mathbf{X}) = \frac{[2\pi^2 \det(\mathbf{B}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp\left[-\pi^2(\mathbf{X} - \hat{\mathbf{X}})^T\mathbf{B}^{-1}(\mathbf{X} - \hat{\mathbf{X}})\right] ; \tag{5.3.5}$$

or if $\mathbf{M}^{-1} = 2\pi^2\mathbf{B}^{-1}$ then

$$\phi(\mathbf{X}) = \frac{\det(\mathbf{M}^{-1})}{(2\pi)^{3/2}} \exp\left[-\tfrac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T\mathbf{M}^{-1}(\mathbf{X} - \hat{\mathbf{X}})\right] , \tag{5.3.6}$$

which is identical to (5.1.3).

5.4 Principal Axis Transformation

The transformation of anisotropic temperature factor coefficients (for the general triclinic case) to principal axes of thermal motion is discussed by Waser,[8] Busing and Levy,[9] and Cruickshank *et al.*[10]

The principal axis transformation is necessary to find the thermal-motion probability ellipsoids discussed in 5.2. The principal axes of the matrix $\mathbf{M}^{-1}$ in (5.3.6) are the vectors $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ for which the inner vector product $(\mathbf{y}_i, \mathbf{y}_i)$ has a stationary value subject to the constraint

$$(\mathbf{y}_i, \mathbf{M}^{-1}\mathbf{y}_i) = 1 , \qquad i = 1, 2, 3 . \tag{5.4.1}$$

For the general triclinic crystal system this means that the quadratic form $\mathbf{y}^T\mathbf{G}^{-1}\mathbf{y}$ has a stationary value subjected to the constraint

$$\mathbf{y}^T\mathbf{G}^{-1}\mathbf{M}^{-1}\mathbf{y} = 1 , \tag{5.4.2}$$

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[8] J. Waser, *Acta Cryst.* **8**, 731 (1955).

[9] W. R. Busing and H. A. Levy, *Acta Cryst.* **11**, 450 (1958).

[10] D. W. J. Cruickshank *et al.*, p. 74 in *Computing Methods and the Phase Problem in X-Ray Crystal Analysis*, ed. by R. Pepinsky, J. M. Robertson, and J. C. Speakman, Pergamon, New York, 1961.

where $\mathbf{G}^{-1}$ is the metric tensor with components $\mathbf{a}_i \cdot \mathbf{a}_j$ and $\mathbf{a}_i \cdot \mathbf{a}_j$ is the scalar vector product of two of the three unit cell vectors. Introducing the Lagrange multiplier $1/\lambda$ leads to

$$\left[\mathbf{G}^{-1} - \frac{1}{\lambda_i} \mathbf{M}^{-1} \right] \mathbf{y}_i = 0 \qquad (i = 1,2,3); \tag{5.4.3}$$

premultiplying by $\mathbf{M}$ yields

$$\left[\mathbf{M}\mathbf{G}^{-1} - \frac{1}{\lambda_i} \mathbf{I} \right] \mathbf{y}_i = 0 \qquad (i = 1,2,3) . \tag{5.4.4}$$

Or we can do some additional rearranging and obtain

$$[\mathbf{G}\mathbf{M}^{-1} - \lambda_i \mathbf{I}] \mathbf{y}_i = 0 \qquad (i = 1,2,3) . \tag{5.4.5}$$

Equation (5.4.4) is equivalent to one of the results derived by Busing and Levy, except the λ_i obtained here are the reciprocals of their λ_i because we are doing the principal axis transformation on $\mathbf{M}^{-1}$ while their formulation performs the transformation on $\mathbf{M}$. The numerical procedure used in OR TEP finds the eigenvalues and eigenvectors of the unsymmetrical matrix $\mathbf{M}\mathbf{G}^{-1}$ in (5.4.4).

6. EXAMPLES OF ILLUSTRATIONS THAT HAVE BEEN PRODUCED WITH OR TEP

Most of the drawings reproduced here were made while OR TEP was under development. Consequently, certain details in the figures are not the same as those produced with the present version of the program. In particular, the lines of shading in the ellipsoid "open octant" are now always evenly spaced.

6.1 Nonsteroscopic Drawings Showing Thermal Motion

The figures in this section have the viewpoint at infinity (parallel projection).

6.1.1 Comparison of Graphical Representations of Thermal Motion. – Figure 6.1 shows the chelation pattern of two citrate molecules related by a twofold screw axis in the crystal structure of magnesium citrate decahydrate.[1] One molecule has "transparent ellipsoids" and the other has "opaque, plugged ellipsoids." Bond types 1, 3, and 4 (see 3.3.9) are illustrated. Note that certain bonds terminate at the ellipsoid boundary while others intersect the ellipsoid. These variables are under the user's control and can be used to advantage for special effects.

Figure 6.2 is another drawing of magnesium citrate decahydrate with the rms magnitudes of displacement along principal axes indicated around the equiprobability thermal ellipsoids.

Figure 6.3 illustrates the same figure with the thermal-motion representation mentioned by Waser,[2] in which the thermal motion is portrayed by a fourth-degree surface generated by a radius vector with length proportional to the rms component of displacement in the direction of the radius vector. The characteristic peanut shape of this fourth-degree surface is most apparent for atom O_3.

The thermal ellipsoid seems to be the preferred representation, and the present version of OR TEP will draw ellipsoids only.

6.1.2 Thermal Ellipsoids Derived from Independent Sets of Diffraction Data. – Figures 6.4(*a*) and (*b*) show the thermal ellipsoids for potassium dihydrogen isocitrate[3] obtained from two independent sets of three-dimensional x-ray data (copper K_α data and chromium K_α data). Figure 6.4(*a*) is presumably a better representation since it is based on a much larger number of measurements. In fact, it is rather surprising that the thermal-motion figures are so similar, considering the limited number of data obtainable with chromium radiation.

6.1.3 Thermal Motion in Molecules Not Related by Crystallographic Symmetry. – Myo-inositol[4] has two molecules in its crystallographic asymmetric unit. Figures 6.5(*a*) and 6.5(*b*) permit a comparison of the two sets of thermal ellipsoids in identical molecular orientations. The hydrogen bonds to neighboring atoms are also indicated. The similarity between the two ellipsoid sets is readily apparent.

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[1] C. K. Johnson, *Acta Cryst.*, in press (1965).

[2] J. Waser, *Acta Cryst.* **8**, 731 (1955).

[3] D. van der Helm, J. P. Glusker, C. K. Johnson, J. A. Minkin, N. E. Burow, and A. L. Patterson, *Acta Cryst.*, in press (1965).

[4] I. N. Rabinowitz and J. Kraut, *Acta Cryst.* **17**, 159 (1964).

6.2 Stereoscopic Drawings of Crystal Structures

6.2.1 Thermal Ellipsoids Derived from Neutron Studies. – Thermal ellipsoids for hydrogen atoms can be derived from neutron diffraction data. Some recent crystal structure results refined from three-dimensional neutron data are shown here as stereoscopic pairs of perspective projections. The thermal ellipsoid for a hydrogen atom is almost always larger than that of the heavier neighbor atom because of zero-point energy.

6.2.1.1 Chloral Hydrate. – Figure 6.6 features two molecules of chloral hydrate[5] related by a center of symmetry. The neighboring hydroxyl groups which are involved in hydrogen bonding to the two molecules are also included.

6.2.1.2 Sugars. – A single molecule of sucrose[6] is shown in Fig. 6.7 with the six-membered glucose ring to the left and the five-membered fructose ring to the right. Two intramolecular hydrogen bonds are drawn between the two moieties. Only one hydroxyl group in the molecule does not form a hydrogen bond; this group has the abnormally large thermal ellipsoid for hydrogen on the left side of the figure.

The thermal motion of a glucose molecule in the α-glucose crystal structure[7] is illustrated by Fig. 6.8. This figure was drawn with OR TEP by G. M. Brown.

6.2.1.3 Lithium Sulphate Monohydrate. – The inorganic structure lithium sulphate monohydrate has been refined with three-dimensional x-ray data by Larson[8] and with three zones of two-dimensional neutron data by Smith and Levy.[9] Figure 6.9 illustrates the characteristic atomic arrangement in that structure. The hydrogen thermal ellipsoids were taken from the neutron analysis and the remainder from the x-ray results. The outstanding feature in this illustration is the large thermal motion of the water molecule, which indicates much looser binding than in the rest of the structure.

6.2.1.4 Potassium Hydrogen Chloromaleate.[10] – This structure contains a centered hydrogen bond. The interatomic bond distances and the surrounding K atoms are also shown in Fig. 6.10, which was drawn with OR TEP by R. D. Ellison and H. A. Levy.

6.2.2 Thermal Ellipsoids Derived from X-Ray Studies. – The examples shown in this section were taken from the literature and from the work of several crystallographers who kindly sent their unpublished results to ORNL to be drawn.

6.2.2.1 Long-Chain Aliphatic Organic Compounds. – Dihydromalvalic acid[11] (cis, D, L-8,9-methylene-heptadecanoic acid) is shown in Fig. 6.11. The thermal motion perpendicular to the chain direction is seen to increase in amplitude toward the nonpolar end of the chain.

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[5] G. M. Brown and H. A. Levy, *Abstracts ACA Meeting, Villanova, Pa.*, H-11 (1962).

[6] G. M. Brown and H. A. Levy, *Science* **141**, 921 (1963).

[7] G. M. Brown and H. A. Levy, *Science* **147**, 1038 (1965).

[8] A. C. Larson, *Acta Cryst.* **18**, 717 (1965).

[9] H. G. Smith and H. A. Levy, *Abstracts ACA Meeting, Boulder, Colorado, 1961.*

[10] R. D. Ellison and H. A. Levy, *Acta Cryst.*, in press (1965).

[11] G. A. Jeffrey and M. Sax, *Acta Cryst.* **16**, 1196 (1963).

Figure 6.12 illustrates the thermal motion in the triglyceride beta-tricaprin.[12] The two molecules shown are related by a center of symmetry. Again the amplitude of motion perpendicular to the chain increases toward the end of the chain.

6.2.2.2 Copper Chelation Compound. – The chelation pattern in *bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II)[13] is demonstrated in Fig. 6.13. The copper atom is on a symmetry center.

6.2.2.3 Large Biological Molecule. – Harunganin,[14] which is a plant pigment, is shown in Fig. 6.14. The pair of "half atoms" at the upper right is an approximation used in the least-squares refinement to correct for either very large thermal motion or disorder which occurs in that part of the crystal structure. The thermal parameters are somewhat questionable since the structure was not refined to convergence. However, the stereogram does permit the molecular configuration to be readily visualized.

6.2.2.4 Abnormal Motion in Cr(III) Acetylacetonate. – Dr. Bruno Morosin from Sandia Corporation sent this most unusual example of thermal motion. Cr(III) acetylacetonate[15] has three acetylacetonate ligands arranged to form an octahedral coordination of oxygens about the Cr atom, as shown in Fig. 6.15. One of the ligands displays very large thermal anisotropy. When a molecular packing diagram such as Fig. 6.16 is viewed, the large displacements are seen to be parallel to the **b** crystal axis. It appears that sheets of these ligands are either disordered or undergoing longitudinal vibration. Morosin has evidence from other diffraction experiments which supports the hypothesis that it is a thermal vibration phenomenon and not static disorder in the crystal.

6.2.3 Crystal Structure Packing Diagrams. – It is often desirable to illustrate the way that molecules pack together in a crystal structure. Sometimes thermal motion can be interpreted on this basis, as was done in 6.2.2.4. In other instances one may be more interested in visualizing the general packing geometry of the crystal structure. Stereograms are very useful for both applications.

6.2.3.1 Potassium Hydrogen Chloromaleate. – A molecule of this structure[10] is shown in Fig. 6.10. Packing diagrams were also drawn by Ellison and Levy and are reproduced here. Figure 6.17 shows the packing of anions about the two types of potassium ions. One coordination polyhedron is an irregular octahedron of oxygen atoms. The other is an irregular 14-hedron having six oxygen atoms and four chlorine atoms at its vertices. Figure 6.18 is a different view of the packing with a larger area included.

6.2.3.2 Packing Diagrams for Inorganic Structures. – The reader may have noticed that most of the illustrations are of organic structures. The reason is that organic molecules are easy to draw. Considerably more planning is required to produce an informative illustration of an inorganic structure.

An approach which is fairly successful is the following:

1. Draw a preliminary stereogram of the contents of a box which encloses somewhat more than one unit cell. Bonds should be drawn in accordance with known interatomic distance ranges. The dimensions

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[12]A. J. Mabis and L. H. Jensen, *Abstracts ACA Meeting, Bozeman, Montana,* F-9 (1964) and L. H. Jensen, private communication, 1964.

[13]G. E. Gurr, *Abstracts ACA Meeting, Bozeman, Montana,* K-7 (1964) and private communication, 1964.

[14]R. A. Alden, G. H. Stout, J. Kraut, and D. F. High, *Acta Cryst.* 17, 109 (1964).

[15]B. Morosin, *Acta Cryst.*, in press (1965) and B. Morosin, private communication, 1964.

for this drawing may be such that the plot can be viewed directly with a stereoscope without photographic reduction.

2. While viewing the preliminary stereogram, pick out the basic structural units and decide on a grouping of these units for the desired figure.

3. Describe the intended subject with whichever technique is the most convenient and draw the new figure. Figure 6.19, potassium perxenate nonahydrate,[16] is an example of an illustration planned in this way. This figure was drawn by J. H. Burns at ORNL.

6.2.3.3 Illustrations of the Contents of a Unit Cell. – A favorite method used by crystallographers is to draw a unit cell outline and the cell contents within that outline. Figure 6.20, which is a stereogram showing lithium α-monodeuteroglycolate,[17] is of this nature. The molecules were kept intact rather than cut off at the cell outline.

6.3 Helical Structures

OR TEP has certain features which facilitate the drawing of nonintegral helical screw models such as those discussed in the field of molecular biology. The Pauling, Corey, and Branson alpha-helix model[18] for protein structure is an example. Figure 6.21 shows the modification of this structure which is present in the synthetic polypeptide poly-L-alanine.[19]

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[16] A. Zalkin, J. D. Forrester, D. H. Templeton, S. M. Williamson, and C. W. Koch, *J. Am. Chem. Soc.* **86**, 3569 (1964).

[17] C. K. Johnson, E. J. Gabe, M. R. Taylor, and I. A. Rose, *J. Am. Chem. Soc.* **87**, 1802 (1965).

[18] L. Pauling, R. B. Corey, and H. R. Branson, *Proc. Natl. Acad. Sci. U.S.* **37**, 235 (1951).

[19] A. Elliott and B. R. Malcolm, *Proc. Roy. Soc. London* **A 249**, 30 (1959).

ORNL DWG. 65-2448

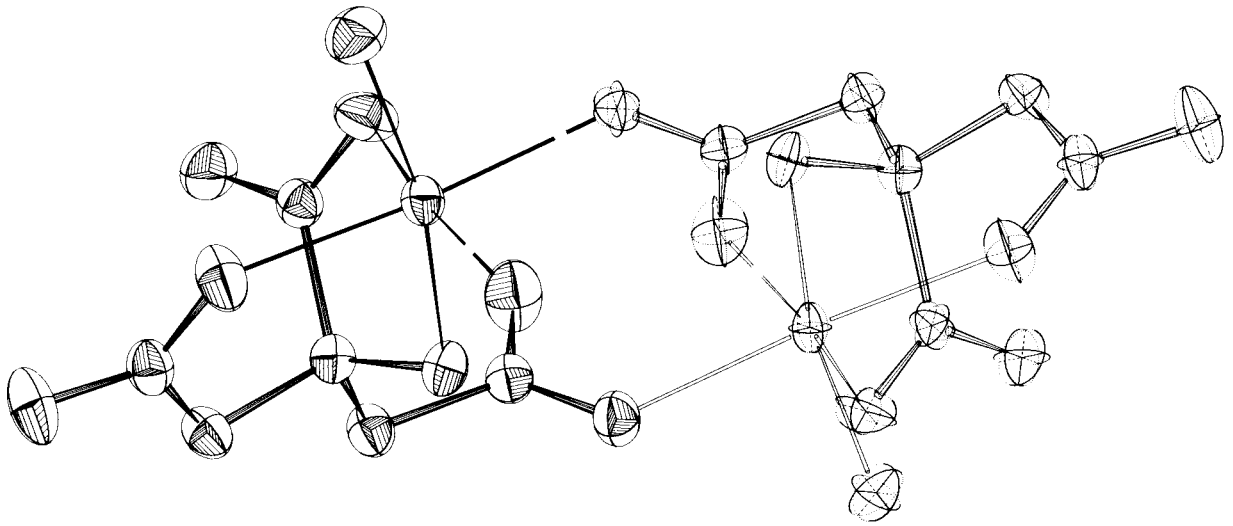

Fig. 6.1. Chelation Pattern Viewed Along a Twofold Screw Axis in the Crystal Structure of Magnesium Citrate Decahydrate. Ellipsoids represent equiprobability surfaces of thermal displacement and contain 65% of the probability distribution.

ORNL DWG. 65-2443

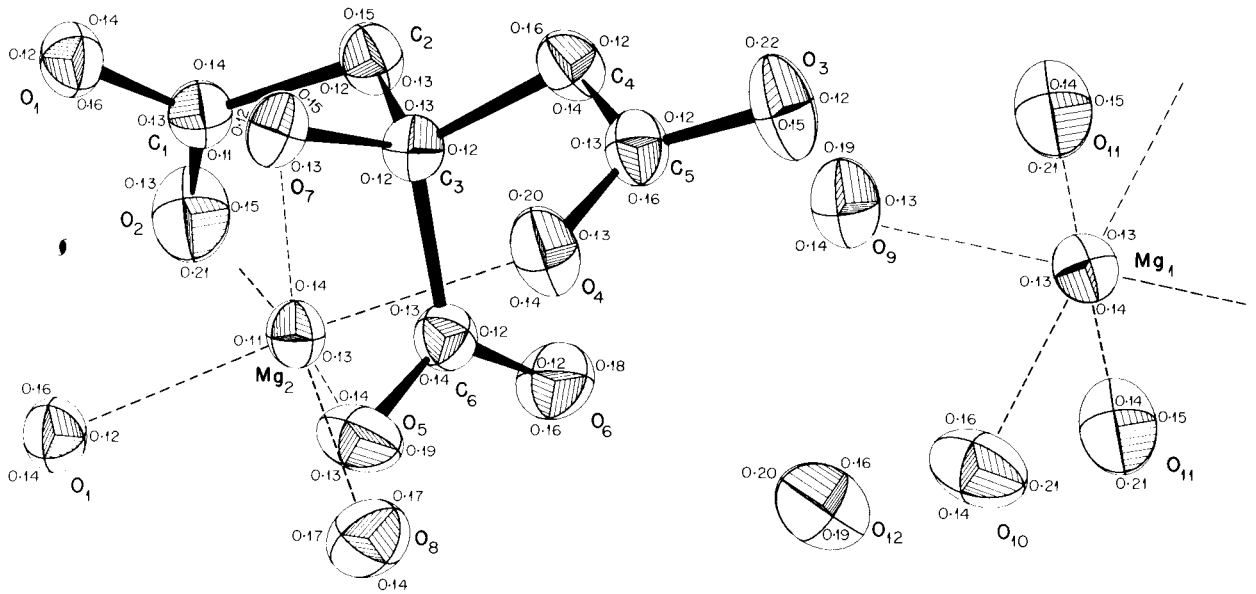

Fig. 6.2. Thermal Ellipsoid Representation for Magnesium Citrate Decahydrate with Principal Values of RMS Displacement in Angstrom Units. Ellipsoids enclose 74% probability. Structure is viewed along *b* axis.

ORNL DWG. 65-2444

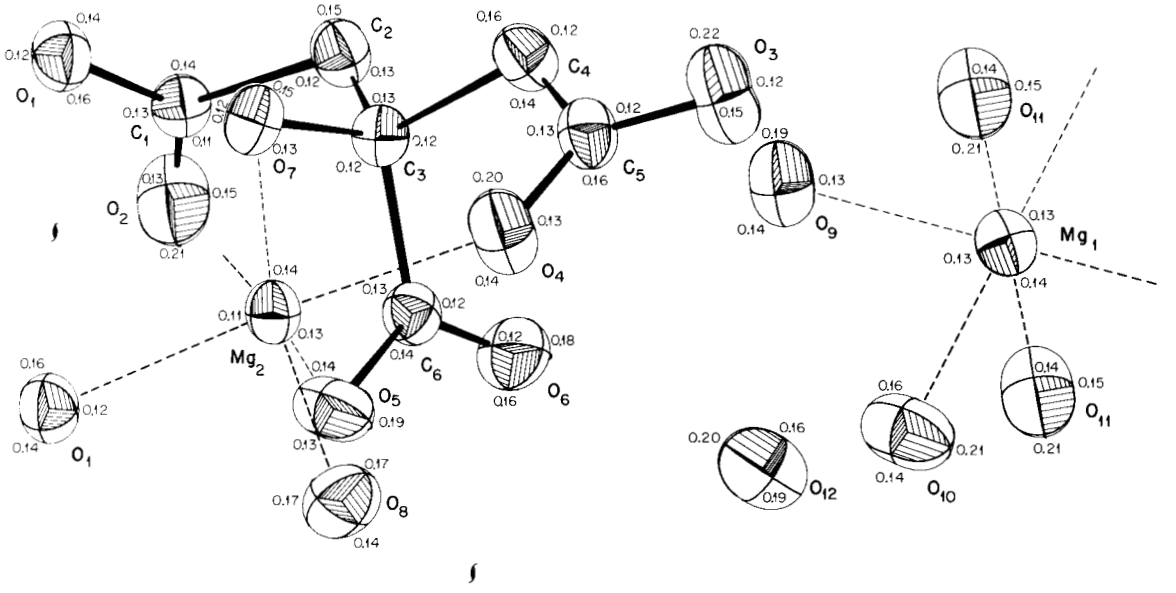

Fig. 6.3. Peanut-Shaped RMS Thermal-Displacement Figure Representation for Magnesium Citrate Decahydrate. Principal values of rms displacement in Angstrom units are indicated around the displacement figures, which are drawn at double scale. Same view of structure as shown in Fig. 6.2.

ORNL DWG. 65-2449

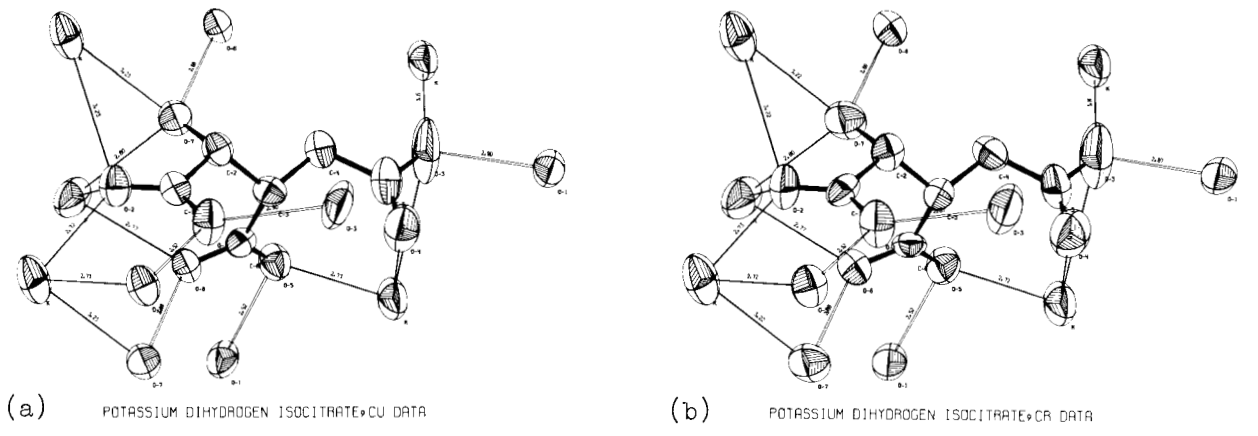

Fig. 6.4. Potassium Dihydrogen Isocitrate with Thermal Ellipsoids Scaled to Include 74% Probability. (*a*) Results obtained from 1350 three-dimensional copper K_α data (disagreement factor 6.5%). (*b*) Results obtained from 340 three-dimensional chromium K_α data (disagreement factor 2.2%). Note: This is *not* a stereo pair.

ORNL DWG. 65-2450

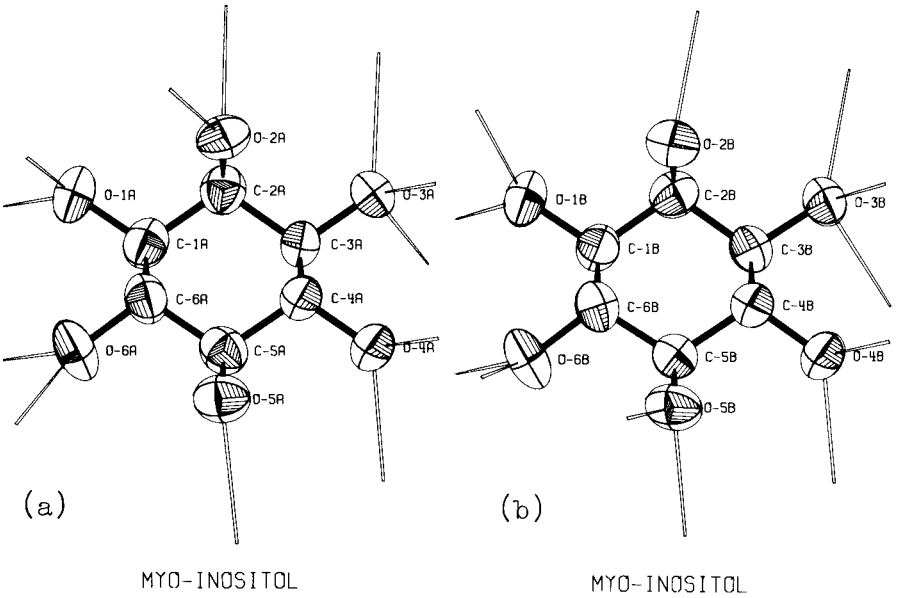

Fig. 6.5. Comparison of Thermal Ellipsoids in the Two Crystallographically Independent Molecules of Myo-Inositol (6.5*a* and 6.5*b*). Hydrogen bonding is shown, since this might influence the thermal motion. Ellipsoids are scaled to include 74% probability. Note: This is *not* a stereo pair.

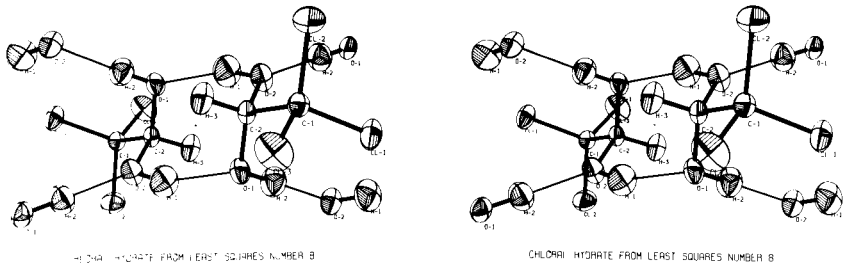

Fig. 6.6. Stereogram (Stereoscopic Pair of Perspective Projections) of Chloral Hydrate Viewed Along the Reciprocal Axis *a.** Two molecules are shown related by a center of symmetry, with the hydrogen bonds connecting them together and to other molecules. Ellipsoids are scaled to include 48% probability.

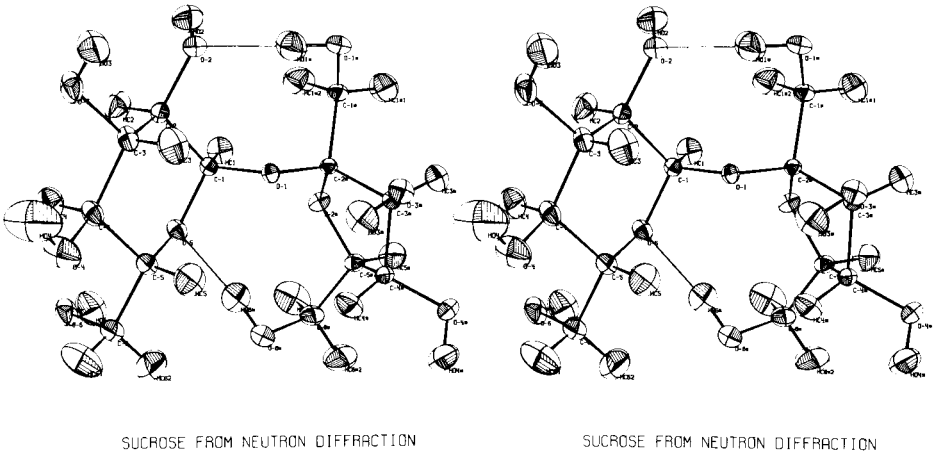

Fig. 6.7. Stereogram Showing the Sucrose Molecule with Thermal Ellipsoids Scaled to Enclose 50% Probability.

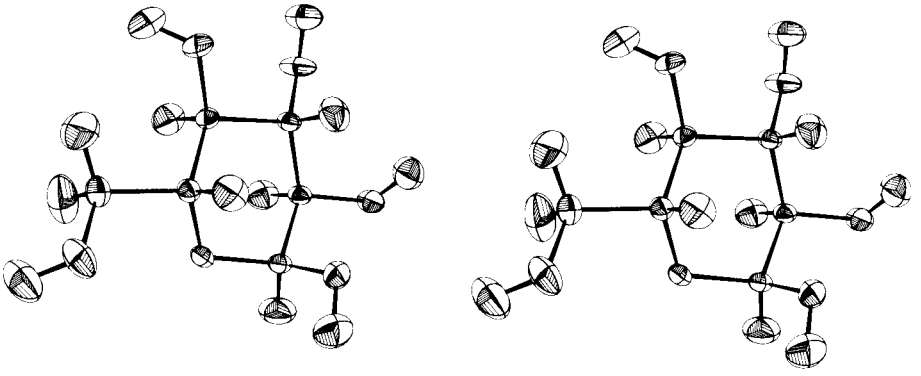

Fig. 6.8. A Molecule of Glucose with Thermal Ellipsoids Scaled to Enclose 50% Probability.

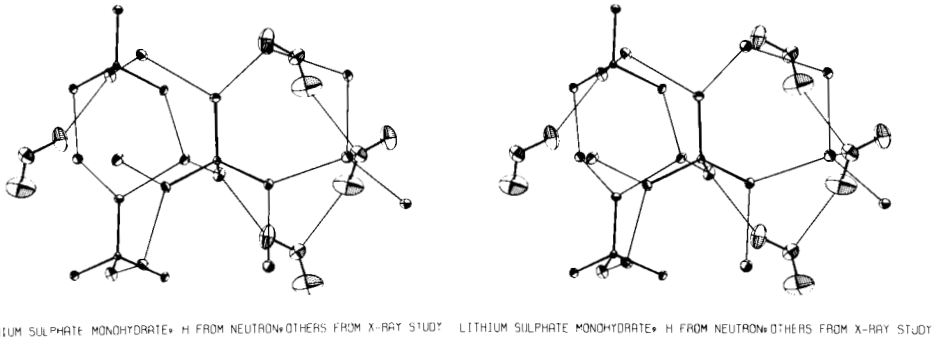

Fig. 6.9. Lithium Sulphate Monohydrate. The lithium ions and sulphate ions are coordinated into a compact network. The structure is viewed along the reciprocal a^* axis. The ellipsoids are scaled to enclose 20% probability.

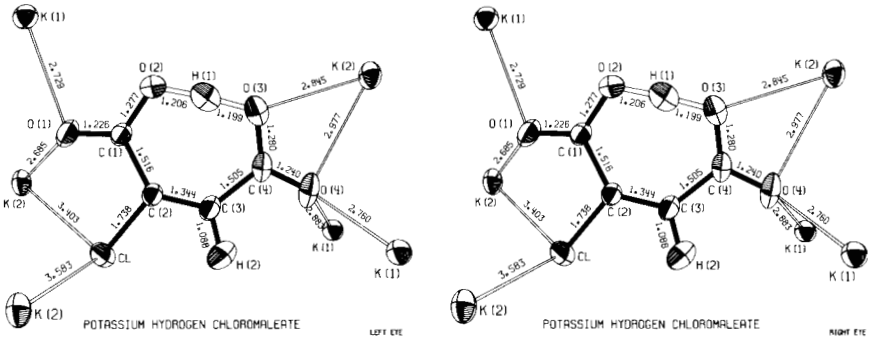

Fig. 6.10. Potassium Hydrogen Chloromaleate. The chloromaleate ion is viewed normal to its own plane. The thermal ellipsoids enclose 50% probability.

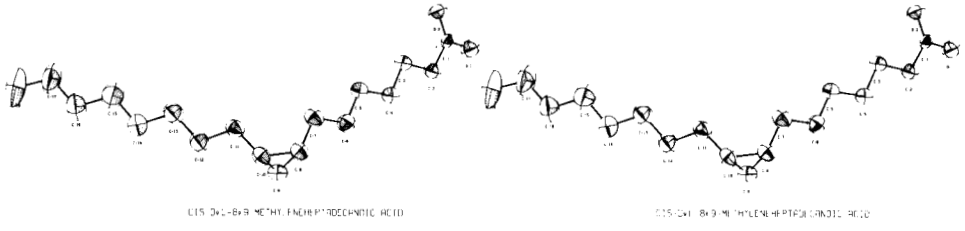

Fig. 6.11. A Molecule of Dihydromalvalic Acid with Thermal Ellipsoids Scaled to Enclose 48% Probability.

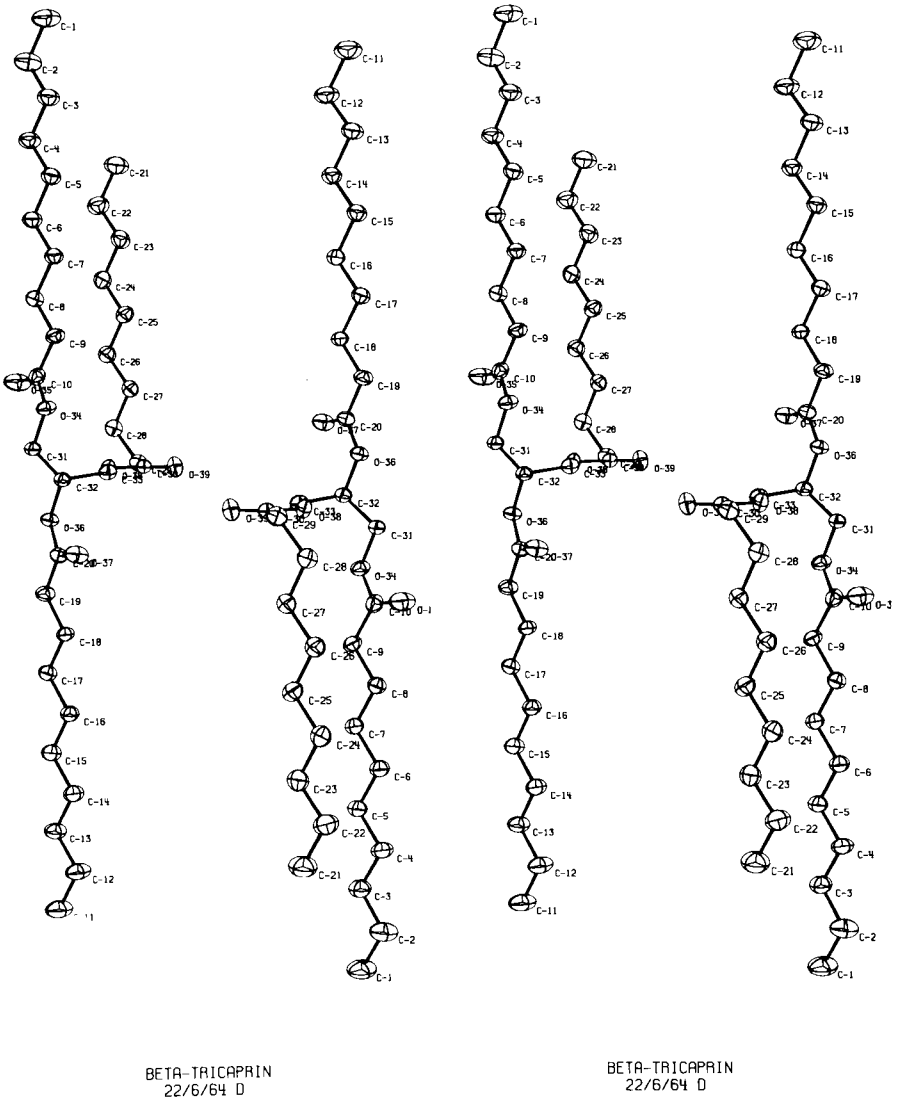

Fig. 6.12. Two Molecules of Beta-Tricaprin Related by a Center of Symmetry. The thermal ellipsoids are scaled to include 30% probability.

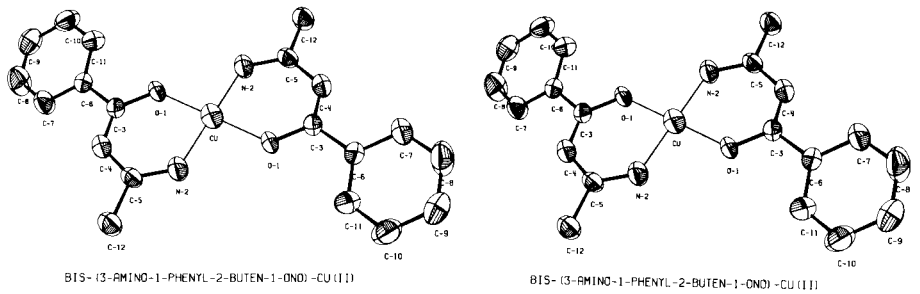

Fig. 6.13. Chelation Complex of *Bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

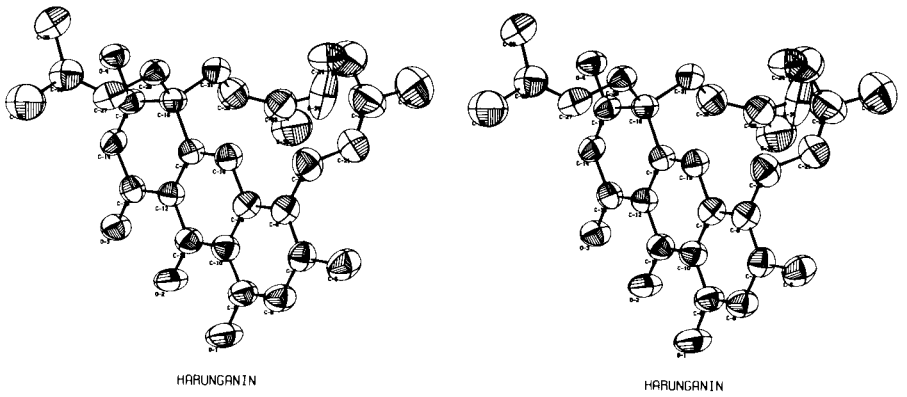

Fig. 6.14. A Molecule of the Plant Pigment Harunganin with Thermal Ellipsoids Scaled to Include 48% Probability.

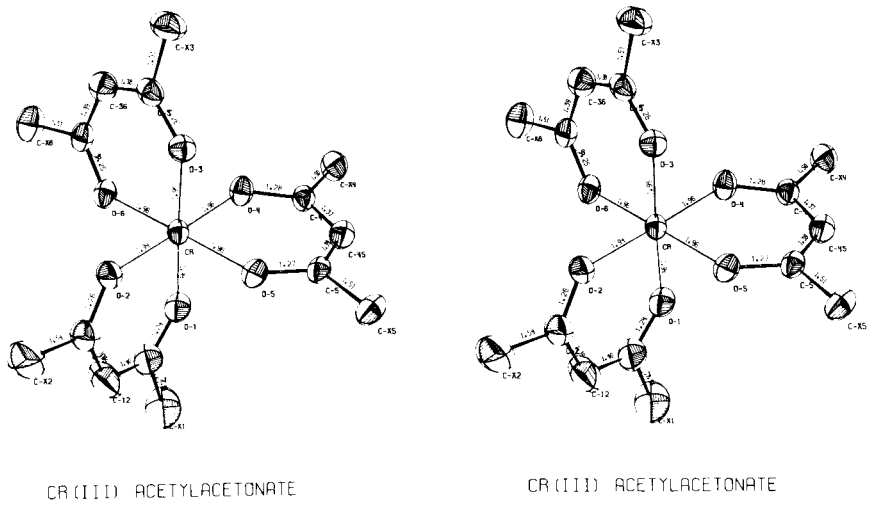

Fig. 6.15. A Unit of *Tris*-acetylacetonatochromium(III) Viewed Along its Threefold Axis of Chemical Symmetry. The thermal ellipsoids are scaled to enclose 20% probability.

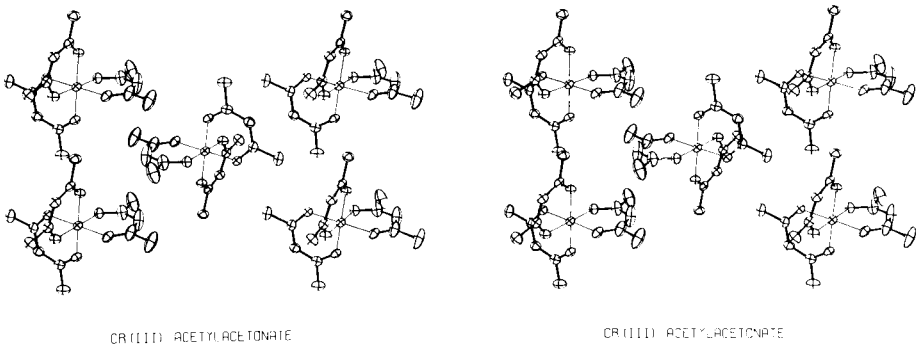

Fig. 6.16. Packing Diagrams for *Tris*-acetylacetonatochromium(III) Viewed Along the Reciprocal Axis c^*. Thermal ellipsoids are scaled to enclose 20% probability.

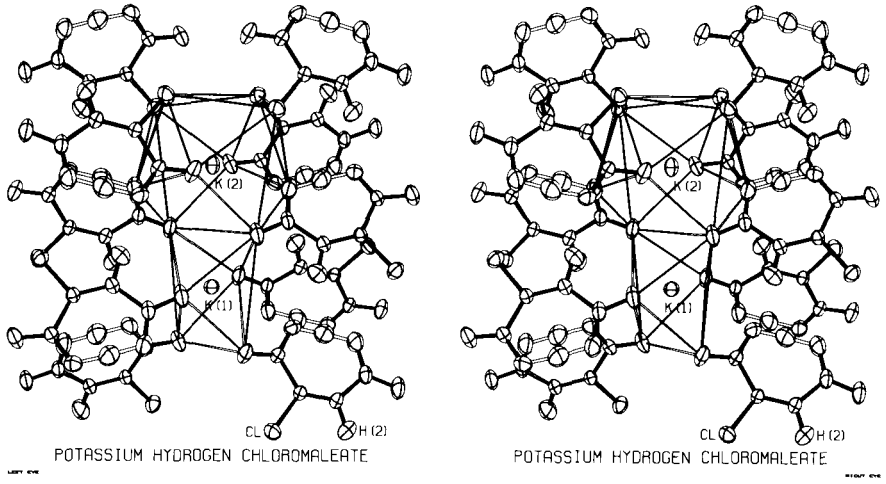

Fig. 6.17. Packing of Chloromaleate Ions Around the Potassium Ions in Potassium Hydrogen Chloromaleate. The edges of the coordination polyhedra are shown. View is nearly along the *c* axis. Thermal ellipsoids are scaled to contain 50% probability.

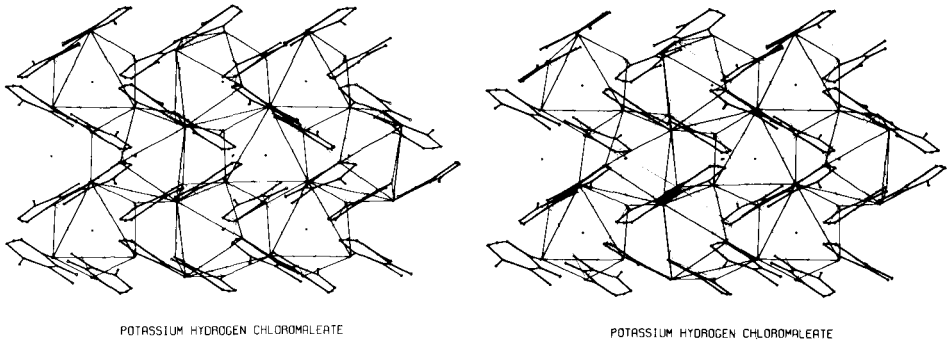

Fig. 6.18. Packing Diagrams for Potassium Hydrogen Chloromaleate. Atoms are represented as small circles. The edges of the coordination polyhedra around the potassium ions are shown. View is nearly along the *a* axis.

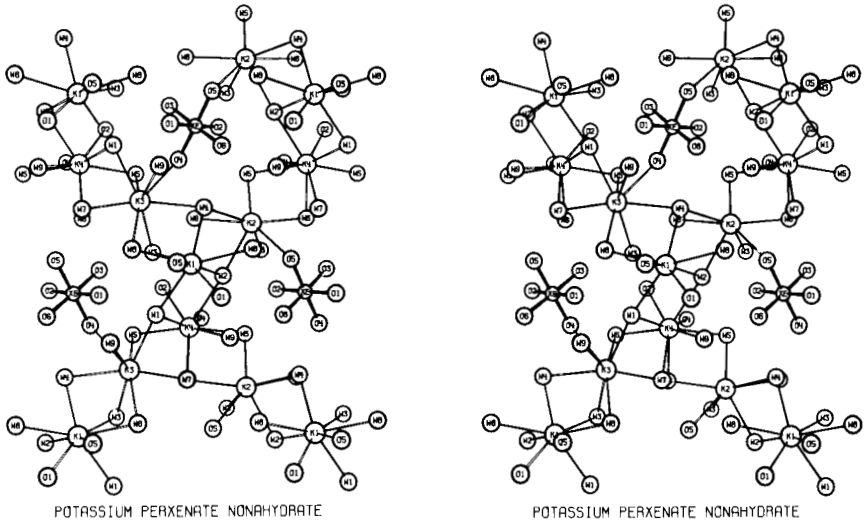

Fig. 6.19. Packing Diagram for Potassium Perxenate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Perxenate Ions. The view is parallel to the *a* axis. Another layer, related to the present one by a twofold screw axis along *a*, is needed to complete the structure.

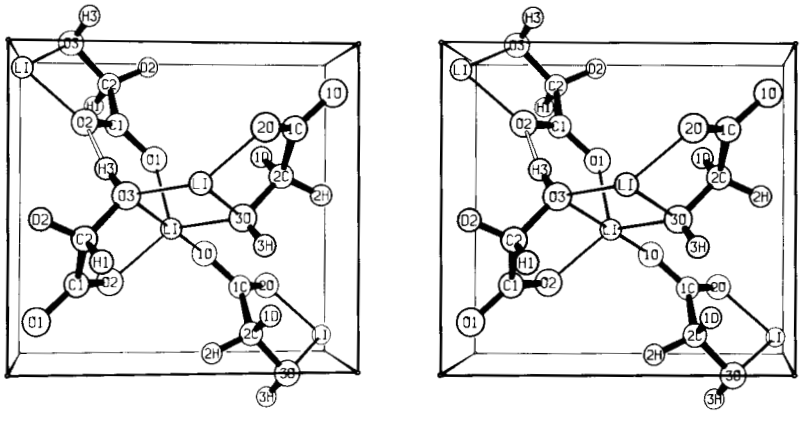

Fig. 6.20. A Stereogram Showing the Unit-Cell Contents of Anhydrous Li α-monodeuteroglycolate. The unique monoclinic *b* axis points up in the page and the mean *c* axis out from the page.

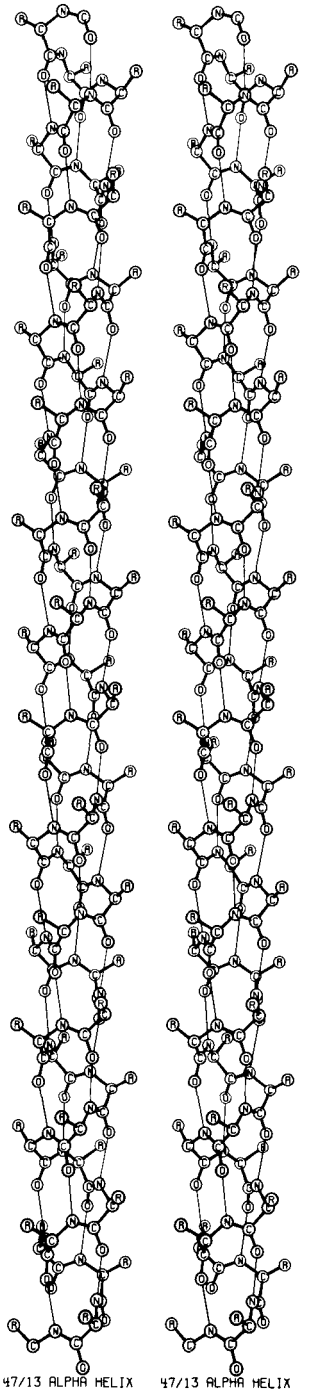

Fig. 6.21. A Stereoscopic Pair of Perspective Projections Showing the Alpha-Helix Which Is Present in Poly-L-Alanine. There are 47 amino-acid residues in 13 turns of the helix. Stereo viewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP

```
*LIST8
*LABEL
CMAIN
C       ***** OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM *****                MAIN0010
        DIMENSICN A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)     MAIN0020
        DIMENSICN ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)MAIN0030
        DIMENSICN DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) MAIN0040
        DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) MAIN0050
        DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   MAIN0060
        DIMENSICN VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   MAIN0070
        DIMENSICN XLNG(3),XO(3),XT(3)                                     MAIN0080
        COMMCN NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   MAIN0090
        COMMCN DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD MAIN0100
        COMMON NJ,NJ2,NOUT,NSR,NSYM,CRGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIMAIN0110
        COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   MAIN0120
        COMMCN V3,V4,V5,V6,WRKV,XLNG,XO,XT                                MAIN0130
      2 CALL PRIME                                                        MAIN0140
C       ***** READ JOB TITLE CARD *****                                   MAIN0150
        READ INPUT TAPE IN,4,(TITLE(I),I#1,12)                            MAIN0160
      4 FORMAT(12A6)                                                      MAIN0170
        WRITE OUTPUT TAPE NOUT,6,(TITLE(I),I#1,12)                        MAIN0180
      5 FORMAT(1H010X,12A6)                                               MAIN0190
      6 FORMAT(1H110X,12A6)                                               MAIN0200
        CALL PRELIM                                                       MAIN0210
        WRITE OUTPUT TAPE NOUT,6,(TITLE(I),I#1,12)                        MAIN0220
        ISAVE#0                                                           MAIN0230
        GO TO 507                                                         MAIN0240
      7 ISAVE#0                                                           MAIN0250
C       ***** ZERO AIN ARRAY *****                                        MAIN0260
      8 DO 10 J#1,140                                                     MAIN0270
     10 AIN(J)#0.                                                         MAIN0280
     11 FORMAT(1H04X,17H(((((( INSTRUCTIONI5,6H ))))))                    MAIN0290
     12 FORMAT(I3,I6,7F9.0)                                               MAIN0300
     13 FORMAT(I3,I6,7E15.8)                                              MAIN0310
     14 FORMAT(1H 9X,7E15.7)                                              MAIN0320
C       ***** READ NEW INSTRUCTICN CARD *****                             MAIN0330
        NCD#0                                                             MAIN0340
        N1#-6                                                             MAIN0350
     16 N1#N1+7                                                           MAIN0360
        N2#N1+6                                                           MAIN0370
        IF(ISAVE)22,18,18                                                 MAIN0380
     18 READ INPUT TAPE IN,12,IC,NF,(AIN(I),I#N1,N2)                      MAIN0390
        IF(ISAVE)24,24,20                                                 MAIN0400
     20 WRITE OUTPUT TAPE NSR,13,IC,NF,(AIN(I),I#N1,N2)                   MAIN0410
        GO TO 24                                                          MAIN0420
     22 READ INPUT TAPE NSR,13,IC,NF,(AIN(I),I#N1,N2)                     MAIN0430
        IF(IC)7,24,24                                                     MAIN0440
     24 IF(N1-1)26,26,30                                                  MAIN0450
     26 WRITE OUTPUT TAPE NOUT,11,NF                                      MAIN0460
        NF1#NF                                                            MAIN0470
        IF(NF1)28,8,30                                                    MAIN0480
     28 IF(NF1+2)2,2,3000                                                 MAIN0490
     30 WRITE OUTPUT TAPE NOUT,14,(AIN(I),I#N1,N2)                        MAIN0500
     32 IC#IC+1                                                           MAIN0510
        GO TO (90,16,38,50),IC                                            MAIN0520
     33 FORMAT(I3,6X,5I3,8F6.0)                                           MAIN0530
     34 FORMAT(6I3,8E12.5)                                                MAIN0540
     35 FORMAT(1H 11X,5I3,8F11.5)                                         MAIN0550
C       ***** READ FORMAT 2 TRAILER CARDS *****                           MAIN0560
     38 NCD#NCD+1                                                         MAIN0570
        IF(ISAVE)44,40,40                                                 MAIN0580
     40 READ INPUT TAPE IN,33,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)      MAIN0590
        IF(ISAVE)46,46,42                                                 MAIN0600
     42 WRITE OUTPUT TAPE NSR,34,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)   MAIN0610
        GO TO 46                                                          MAIN0620
     44 READ INPUT TAPE NSR,34,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)     MAIN0630
     46 WRITE OUTPUT TAPE NOUT,35,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)     MAIN0640
        GO TO 32                                                          MAIN0650
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C     ***** READ FORMAT 3 TRAILER CARD *****                          MAIN0660
   50 INN#IN                                                          MAIN0670
      IF(ISAVE)52,54,54                                               MAIN0680
   52 INN#NSR                                                         MAIN0690
   54 READ INPUT TAPE INN,4,(TITLE2(I),I#1,12)                        MAIN0700
      WRITE OUTPUT TAPE NOUT,5,(TITLE2(I),I#1,12)                     MAIN0710
      IF(ISAVE)90,90,56                                               MAIN0720
   56 WRITE OUTPUT TAPE NSR,4,(TITLE2(I),I#1,12)                      MAIN0730
C     ***** EXECUTE INSTRUCTION *****                                 MAIN0740
   90 NJ#NF1/100                                                      MAIN0750
      NJ2#NF1-NJ*100                                                  MAIN0760
      NJ3#XMODF(NJ2,10)                                               MAIN0770
      IF(NJ-12)98,92,92                                               MAIN0780
   92 CALL SPARE(NF1)                                                 MAIN0790
      IF(NG)94,8,94                                                   MAIN0800
   94 CALL ERPNT(0.,NF1)                                              MAIN0810
      GO TO 8                                                         MAIN0820
C     ******BRANCH TABLE FOR FUNCTION TYPES******                     MAIN0830
   98 GO TO(100,200,300,400,500,600,700,800,900,1000,1100),NJ         MAIN0840
C     *******STRUCTURE ANALYSIS FUNCTIONS*******                      MAIN0850
  100 GO TO (101,101,104,104,94),NJ2                                  MAIN0860
  101 CALL SEARCH                                                     MAIN0870
      GO TO 8                                                         MAIN0880
C     ***** ANISOTROPIC TEMP FACTOR OUTPUT *****                      MAIN0890
  104 DO 164 I#1,NATOM                                                MAIN0900
      IF(XMODF(I,14)-1)134,114,134                                    MAIN0910
  114 WRITE OUTPUT TAPE NOUT,6,(TITLE(J),J#1,12)                      MAIN0920
      WRITE OUTPUT TAPE NOUT,129                                      MAIN0930
  129 FORMAT(1H0 10X,4HATOM3X,16HRMS DISPLACEMENT3X,31HROW VECTORS, BASEDMAIN0940
     1 ON REFERENCE17X,29HPROBABILITY COVARIANCE MATRIX)              MAIN0950
  134 TI#55501.+FLOATF(I)*100000.                                     MAIN0960
      CALL PAXES(TI,-3)                                               MAIN0970
      IF(NG)144,154,144                                               MAIN0980
  144 CALL ERPNT(TI,104)                                              MAIN0990
  149 FORMAT(1H0 10X,A6,F10.6,6X,3F12.7,10X,3F12.7)                   MAIN1000
  154 WRITE OUTPUT TAPE NOUT,149,CHEM(I),RMS(I),(PAC(J,I),J#1,3),(Q(J,I)MAIN1010
     1,J#1,3)                                                         MAIN1020
  164 WRITE OUTPUT TAPE NOUT,159,(RMS(K),(PAC(J,K),J#1,3),(Q(J,K),J#1,3)MAIN1030
     1,K#2,3)                                                         MAIN1040
  159 FORMAT(1H 16X,F10.6,6X,3F12.7,10X,3F12.7)                       MAIN1050
      GO TO 8                                                         MAIN1060
C     *******PLOTTER INITIALIZE,FRAME ADVANCE,TERMINATE FUNCTIONS*******MAIN1070
  200 CALL F200                                                       MAIN1080
      GO TO 8                                                         MAIN1090
  300 GO TO (301,302,303,94),NJ2                                      MAIN1100
C     *******PLOT DIMENSIONS******                                    MAIN1110
  301 IF(AIN(1))321,321,311                                           MAIN1120
  311 XLNG(1)#AIN(1)                                                  MAIN1130
  321 IF(AIN(2))341,341,331                                           MAIN1140
  331 XLNG(2)#AIN(2)                                                  MAIN1150
  341 IF(AIN(3))361,361,351                                           MAIN1160
  351 VIEW#AIN(3)                                                     MAIN1170
  361 IF(AIN(4))381,381,371                                           MAIN1180
  371 BRDR#AIN(4)                                                     MAIN1190
  381 WRITE OUTPUT TAPE NOUT,389,XLNG(1),XLNG(2),BRDR                 MAIN1200
  389 FORMAT(1H0 10X,11HPLOT LIMITSF6.2,3H BYF6.2,15H IN.  INCLUDINGF6.2,MAIN1210
     112H  IN. MARGIN)                                                MAIN1220
  391 WRITE OUTPUT TAPE NOUT,399,VIEW                                 MAIN1230
  399 FORMAT(1H 10X,13HVIEW DISTANCEF7.3,7H INCHES)                   MAIN1240
      GO TO 8                                                         MAIN1250
C     *******LEGEND ROTATION*******                                   MAIN1260
  302 THETA#AIN(1)                                                    MAIN1270
      TI#THETA*.01745329252                                           MAIN1280
      COSTH#COSF(TI)                                                  MAIN1290
      SINTH#SINF(TI)                                                  MAIN1300
      DO 312 J#1,9                                                    MAIN1310
  312 SYMB(J,1)#0.                                                    MAIN1320
      SYMB(1,1)#COSTH                                                 MAIN1330
      SYMB(2,2)#COSTH                                                 MAIN1340
      SYMB(3,3)#1.                                                    MAIN1350
```

```
      SYMB(2,1)#SINTH                                                   MAIN1360
      SYMB(1,2)#-SINTH                                                  MAIN1370
      WRITE OUTPUT TAPE NOUT,319,THETA                                  MAIN1380
  319 FORMAT(1H01OX,44HREGULAR TITLE AND SYMBOL ROTATION IN DEGREESF8.2)MAIN1390
      GO TO 8                                                           MAIN1400
C     ***** RETRACE DISPLACEMENT *****                                  MAIN1410
  303 DISP#AIN(1)                                                       MAIN1420
      WRITE OUTPUT TAPE NOUT,313,DISP                                   MAIN1430
  313 FORMAT(1H01OX,22HRETRACE DISPLACEMENT #F7.4,5H INCH)              MAIN1440
      GO TO 8                                                           MAIN1450
C     *******ATOM LIST FUNCTIONS******                                  MAIN1460
  400 GO TO (401,401,401,490,94,94,94,94,94,410,401,401,401,94),NJ2     MAIN1470
  401 CALL F400                                                         MAIN1480
      GO TO 490                                                         MAIN1490
  410 LATM#0                                                            MAIN1500
      DO 420 I#1,500                                                    MAIN1510
      DO 420 J#1,4                                                      MAIN1520
  420 ATCMS(J,I)#0.                                                     MAIN1530
  490 IF(LATM)8,8,491                                                   MAIN1540
  491 WRITE OUTPUT TAPE NOUT,499,(ATOMS(1,I),I#1,LATM)                  MAIN1550
  499 FORMAT(1H01OX,23HCCNTENTS OF ATOMS ARRAY/(15X,10F10.0))           MAIN1560
      GO TO 8                                                           MAIN1570
C     *******CARTESIAN COORDINATE SYSTEM FUNCTIONS*******               MAIN1580
  500 CALL F500                                                         MAIN1590
      IF(NJ3-3)507,539,539                                              MAIN1600
  507 WRITE OUTPUT TAPE NOUT,529                                        MAIN1610
      WRITE OUTPUT TAPE NOUT,519,((REFV(J,I),I#1,3),(AAREV(J,I),I#1,3),JMAIN1620
     1#1,3)                                                             MAIN1630
      GO TO 8                                                           MAIN1640
  509 FORMAT(1H01OX, 49HORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXEMAIN1650
     1S18X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VECMAIN1660
     2TOR8X,8HZ VECTOR)                                                 MAIN1670
  519 FORMAT(1H 10X,3E16.7,8X,3E16.7)                                   MAIN1680
  529 FORMAT(1H01OX,51HORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXMAIN1690
     1ES16X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VEMAIN1700
     2CTOR8X,8HZ VECTOR)                                                MAIN1710
  539 WRITE OUTPUT TAPE NOUT,509                                        MAIN1720
      WRITE OUTPUT TAPE NOUT,519,((WRKV(J,I),I#1,3),(AAWRK(J,I),I#1,3),JMAIN1730
     1#1,3)                                                             MAIN1740
      GO TO 8                                                           MAIN1750
C     *******PLOT CENTERING FUNCTIONS*******                            MAIN1760
  600 CALL F600                                                         MAIN1770
      WRITE OUTPUT TAPE NOUT,609,XO(1),XO(2),SCAL1,SCAL2                MAIN1780
  609 FORMAT(1H01OX,31HORIGIN POINT IN PLOTTER COORD.(F6.2,2H ,F6.2,8H )MAIN1790
     1 IN.  / 11X,15HOVERALL SCALE #F6.3,32H INCH/ANGSTROM ELLIPSOID SCAMAIN1800
     2LE #F6.3)                                                         MAIN1810
      GO TO 391                                                         MAIN1820
C     *******ELLIPSOID AND SYMBOL PLOT FUNCTIONS*******                 MAIN1830
C     ********FILL OUT DETAILS FOR SPECIAL MODELS********               MAIN1840
  700 GO TO (701,702,704,705,709,94),NJ3                                MAIN1850
  701 AIN(3)#8.                                                         MAIN1860
      GO TO 703                                                         MAIN1870
  702 AIN(3)#0.                                                         MAIN1880
  703 AIN(1)#4.                                                         MAIN1890
      AIN(2)#0.                                                         MAIN1900
      AIN(4)#0.                                                         MAIN1910
      GO TO 709                                                         MAIN1920
  704 AIN(1)#3.                                                         MAIN1930
      AIN(2)#-5.                                                        MAIN1940
      GO TO 706                                                         MAIN1950
  705 AIN(1)#1.                                                         MAIN1960
      AIN(2)#0.                                                         MAIN1970
  706 AIN(3)#1.                                                         MAIN1980
      AIN(4)#5.                                                         MAIN1990
  709 CALL F700                                                         MAIN2000
      GO TO 8                                                           MAIN2010
C     *******8CND FUNCTIONS*******                                      MAIN2020
  800 CALL F800                                                         MAIN2030
      GO TO 8                                                           MAIN2040
C     *******TITLE FUNCTICNS*******                                     MAIN2050
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  900 CALL F900                                                         MAIN2060
      GO TO 8                                                           MAIN2070
C     *******CELL OUTLINE FUNCTIONS*******                              MAIN2080
 1000 CALL F1000                                                        MAIN2090
      GO TO 8                                                           MAIN2100
C     *******SAVE SEQUENCE FUNCTIONS*******                             MAIN2110
 1100 IF(NJ2-2)1101,1102,1103                                           MAIN2120
 1101 ISAVE#1                                                           MAIN2130
      GO TO 1104                                                        MAIN2140
 1102 ISAVE#0                                                           MAIN2150
      J#-1                                                              MAIN2160
      WRITE OUTPUT TAPE NSR,13,J,NF1,(AIN(I),I#1,7)                     MAIN2170
      END FILE NSR                                                      MAIN2180
      GO TO 1104                                                        MAIN2190
 1103 ISAVE#-1                                                          MAIN2200
 1104 REWIND NSR                                                        MAIN2210
      GO TO 8                                                           MAIN2220
 3000 CALL EXIT                                                         MAIN2230
      END                                                               MAIN2240
*LIST8
*LABEL
      FUNCTION ARCCOS(X)                                                ARCC0010
C     ARCCOS(X) IN DEGREES                                              ARCC0020
      IF(1.0-ABSF(X))1,2,2                                              ARCC0030
    1 X#SIGNF(1.0,X)                                                    ARCC0040
    2 IF(X)3,4,5                                                        ARCC0050
    3 ARCCOS#180.0+ATANF(SQRTF(1.0-X*X)/X)*57.29577951                  ARCC0060
      GO TO 6                                                           ARCC0070
    4 ARCCOS#90.0                                                       ARCC0080
      GO TO 6                                                           ARCC0090
    5 ARCCOS#ATANF(SQRTF(1.0-X*X)/X)*57.29577951                        ARCC0100
    6 RETURN                                                            ARCC0110
      END                                                               ARCC0120
*LIST8
*LABEL
      SUBROUTINE ATOM(QA,Z)                                             ATOM0010
C     ATOM COORDINATE SUBROUTINE                                        ATOM0020
      DIMENSION X(3),Z(3)                                               ATOM0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ATOM0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)ATOM0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) ATOM0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ATOM0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   ATOM0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ATOM0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     ATOM0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ATOM0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ATOM0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIATOM0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ATOM0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ATOM0150
      K#QA/100000.0                                                     ATOM0160
      IF(K)109,109,117                                                  ATOM0170
  109 X(1)#0.0                                                          ATOM0180
      X(2)#0.0                                                          ATOM0190
      X(3)#0.0                                                          ATOM0200
      GO TO 125                                                         ATOM0210
  117 IF(K-NATOM)119,119,503                                            ATOM0220
  503 NG#5                                                              ATOM0230
      GO TO 325                                                         ATOM0240
  119 DO123J#1,3                                                        ATOM0250
  123 X(J)#P(J,K)                                                       ATOM0260
  125 TA#ABSF(QA)                                                       ATOM0270
      KSYM#MODF(TA,100000.0)                                            ATOM0280
      KT#KSYM/100                                                       ATOM0290
      KS#KSYM-100*KT                                                    ATOM0300
      IF(KS-NSYM)203,203,403                                            ATOM0310
  403 NG#4                                                              ATOM0320
      GO TO 325                                                         ATOM0330
  203 IF(KS)403,205,213                                                 ATOM0340
  205 Z(1)#X(1)                                                         ATOM0350
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      Z(2)#X(2)                                                         ATOM0360
      Z(3)#X(3)                                                         ATOM0370
      GO TO 311                                                         ATOM0380
  213 DO 223 K#1,3                                                      ATOM0390
      Z(K)#TS(K,KS)                                                     ATOM0400
      DO 223 J#1,3                                                      ATOM0410
  223 Z(K)#Z(K)+FS(J,K,KS)*X(J)                                         ATOM0420
  311 IF(KT)403,325,313                                                 ATOM0430
  313 IF(KT-555)317,315,317                                             ATOM0440
  315 KSYM#KS                                                           ATOM0450
      GO TO 325                                                         ATOM0460
  317 K1#KT/100                                                         ATOM0470
      K#KT-100*K1                                                       ATOM0480
      K2#K/10                                                           ATOM0490
      K3#K-10*K2                                                        ATOM0500
      Z(1)#Z(1)+FLOATF(K1-5)                                            ATOM0510
      Z(2)#Z(2)+FLOATF(K2-5)                                            ATOM0520
      Z(3)#Z(3)+FLOATF(K3-5)                                            ATOM0530
  325 RETURN                                                            ATOM0540
      END                                                               ATOM0550
*LIST8
*LABEL
      SUBROUTINE AXEQB(A1,X,B1,JJJ)                                     AXEQ0010
C     ***** SOLUTION OF MATRIX EQUATION AX#B FOR X *****                AXEQ0020
C     ***** USES METHOD OF TRIANGULAR ELIMINATION *****                 AXEQ0030
C     ***** B AND X HAVE DIMENSIONS (3,JJJ),A IS ALWAYS (3,3)           AXEQ0040
C     ***** TO INVERT A MAKE B 3 BY 3 IDENITY MATRIX *****              AXEQ0050
      DIMENSION A1(3,3),A(3,3),B(3,3),B1(3,3),X(3,3)                    AXEQ0060
      NV#JJJ                                                            AXEQ0070
C     ***** TRANSFER DATA *****                                         AXEQ0080
      DO 2 I#1,3                                                        AXEQ0090
      DO 2 J#1,3                                                        AXEQ0100
      IF(NV-J)2,1,1                                                     AXEQ0110
    1 B(I,J)#B1(I,J)                                                    AXEQ0120
    2 A(I,J)#A1(I,J)                                                    AXEQ0130
C     ***** TRIANGULARIZE MATRIX A *****                                AXEQ0140
      DO 17 I#1,2                                                       AXEQ0150
      S#0.0                                                             AXEQ0160
      DO 4 J#I,3                                                        AXEQ0170
      R#ABSF(A(J,I))                                                    AXEQ0180
      IF(R-S)4,3,3                                                      AXEQ0190
    3 S#R                                                               AXEQ0200
      L#J                                                               AXEQ0210
    4 CONTINUE                                                          AXEQ0220
      IF(L-I)5,10,5                                                     AXEQ0230
    5 DO 6 J#I,3                                                        AXEQ0240
      S#A(I,J)                                                          AXEQ0250
      A(I,J)#A(L,J)                                                     AXEQ0260
    6 A(L,J)#S                                                          AXEQ0270
      DO 8 J#1,NV                                                       AXEQ0280
      S#B(I,J)                                                          AXEQ0290
      B(I,J)#B(L,J)                                                     AXEQ0300
    8 B(L,J)#S                                                          AXEQ0310
   10 TEM#A(I,I)                                                        AXEQ0320
      IF(TEM)11,17,11                                                   AXEQ0330
   11 IPO#I+1                                                           AXEQ0340
      DO 16 J#IPO,3                                                     AXEQ0350
      IF(A(J,I))12,16,12                                                AXEQ0360
   12 S#A(J,I)/TEM                                                      AXEQ0370
      A(J,I)#0.0                                                        AXEQ0380
      DO 13 K#IPO,3                                                     AXEQ0390
   13 A(J,K)#A(J,K)-A(I,K)*S                                            AXEQ0400
      DO 15 K#1,NV                                                      AXEQ0410
   15 B(J,K)#B(J,K)-B(I,K)*S                                            AXEQ0420
   16 CONTINUE                                                          AXEQ0430
   17 CONTINUE                                                          AXEQ0440
C     ***** MODIFY SINGULAR MATRIX *****                                AXEQ0450
      DO 20 I#1,3                                                       AXEQ0460
      IF(A(I,I))20,19,20                                                AXEQ0470
   19 A(I,I)#MAX1F(1.E-25,MAX1F(A(1,1),A(2,2),A(3,3))*1.E-15)           AXEQ0480
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   20 CONTINUE                                                          AXEQ0490
      DO 24 K#1,NV                                                      AXEQ0500
      DO 24 I#1,3                                                       AXEQ0510
      N#4-I                                                             AXEQ0520
      M#N+1                                                             AXEQ0530
      TEM#B(N,K)                                                        AXEQ0540
      IF(3-M)23,21,21                                                   AXEQ0550
   21 DO 22 J#M,3                                                       AXEQ0560
   22 TEM#TEM-A(N,J)*B(J,K)                                             AXEQ0570
   23 B(N,K)#TEM/A(N,N)                                                 AXEQ0580
   24 X(N,K)#B(N,K)                                                     AXEQ0590
      RETURN                                                            AXEQ0600
      END                                                               AXEQ0610
*LIST8
*LABEL
      SUBROUTINE AXES(U,V,X,ITYPE)                                      AXES0010
C     ***** STORE THREE ORTHOGONAL VECTORS EACH 1 ANGSTROM LONG *****   AXES0020
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         AXES0030
C     ***** XABSF(ITYPE)#1 W(1)#U,W(2)#(UXV),W(3)#UX(UXV) *****         AXES0040
C     ***** XABSF(ITYPE)#2 W(1)#U,W(2)#(UXV)XU,W(3)#(UXV) *****         AXES0050
C     ***** ITYPE#0 W(1)#A,W(2)#(AXB)XA,W(3)#(AXB), ABC#CELL VECTORS ***AXES0060
      DIMENSION U(3),V(3),W(3,3),X(3,3)                                 AXES0070
      IT#ITYPE                                                          AXES0080
      IF(IT)115,105,115                                                 AXES0090
  105 U(1)#1.                                                           AXES0100
      U(2)#0.                                                           AXES0110
      U(3)#0.                                                           AXES0120
      V(1)#0.                                                           AXES0130
      V(2)#1.                                                           AXES0140
      V(3)#0.                                                           AXES0150
  115 DO 125 J#1,3                                                      AXES0160
  125 W(J,1)#U(J)                                                       AXES0170
      IF(XABSF(IT)-1)145,135,145                                        AXES0180
  135 CALL NORM(U,V,W(1,2),IT)                                          AXES0190
      CALL NORM(U,W(1,2),W(1,3),IT)                                     AXES0200
      GO TO 155                                                         AXES0210
  145 CALL NORM(U,V,W(1,3),IT)                                          AXES0220
      CALL NORM(W(1,3),U,W(1,2),IT)                                     AXES0230
  155 DO 195 I#1,3                                                      AXES0240
      IF(IT)165,165,175                                                 AXES0250
  165 IC#-1                                                             AXES0260
      GO TO 195                                                         AXES0270
  175 IC#1                                                              AXES0280
  195 CALL UNIT(W(1,I),X(1,I),IC)                                       AXES0290
      RETURN                                                            AXES0300
      END                                                               AXES0310
*LIST8
*LABEL
      SUBROUTINE BOND(Z1,Z2,NB)                                         BOND0010
      DIMENSION B(3,3),E(3,3),R(3,3),RT(3,3),S(3,3),U(3,3),VUE(3)       BOND0020
      DIMENSION V7(3),W(13,2),X(3),Z(3)                                 BOND0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    BOND0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)BOND0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) BOND0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) BOND0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   BOND0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   BOND0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     BOND0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   BOND0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATN,LTNO,NATOM,NCD BOND0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIBOND0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   BOND0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                BOND0150
C     ***** OBTAIN POSITIONAL PARAMETERS *****                          BOND0160
      NG1#0                                                             BOND0170
      DO 105 J#1,26                                                     BOND0180
  105 W(J,1)#0.                                                         BOND0190
      W(1,1)#Z1                                                         BOND0200
      W(1,2)#Z2                                                         BOND0210
      DO 135 I#1,2                                                      BOND0220
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      CALL XYZ(W(1,I),W(4,I),2)                                         BOND0230
      IF(NG)125,110,125                                                 BOND0240
  110 DO 115 J#1,3                                                      BOND0250
  115 W(J+6,I)#XT(J)                                                    BOND0260
      K#W(1,I)/100000.                                                  BOND0270
      L#W(1,I)-FLOATF(K)*100000.                                        BOND0280
      CALL PLTXY(W(4,I),W(2,I))                                         BOND0290
      IF(EDGE-BRDR*.25)120,128,128                                      BOND0300
  120 NG#10                                                             BOND0310
  125 NG1#1                                                             BOND0320
      WRITE OUTPUT TAPE NOUT,136,CHEM(K),K,L,(W(J,I),J#2,9)             BOND0330
      CALL ERPNT(W(1,I),800)                                            BOND0340
      GO TO 135                                                         BOND0350
  128 IF(NJ2-10)130,135,135                                             BOND0360
  130 WRITE OUTPUT TAPE NOUT,136,CHEM(K),K,L,(W(J,I),J#2,9)             BOND0370
  135 CONTINUE                                                          BOND0380
  136 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)   2F8.2,5X,3F8.3,13X,3F8.4)    BOND0390
      IF(NG1)999,140,999                                                BOND0400
  140 CALL DIFV(W(7,1),W(7,2),V7)                                       BOND0410
      DIST#SQRTF(VMV(V7,AA,V7))                                         BOND0420
      IF(XMODF(NJ2,10)-3)143,142,142                                    BOND0430
  142 HGT#SCAL1*.12                                                     BOND0440
      CALL SIMBOL(W(2,1),W(3,1),HGT,XMODF(XFIXF(W(1,1)/100000.),10),0.,-BOND0450
     11)                                                                BOND0460
      CALL SIMBOL(W(2,2),W(3,2),HGT,XMODF(XFIXF(W(1,2)/100000.),10),0.,-BOND0470
     12)                                                                BOND0480
      GO TO 570                                                         BOND0490
  143 KODE#KD(5,NB)                                                     BOND0500
      IF(KODE)145,144,146                                               BOND0510
  144 NBND#0                                                            BOND0520
      GO TO 148                                                         BOND0530
  145 KODE#-KODE                                                        BOND0540
  146 NBND#128/2**KODE                                                  BOND0550
C     ***** FIND UPPERMOST ATOM PUT IN POSITION ONE *****               BOND0560
  148 IF(VIEW)152,150,152                                               BOND0570
  150 W(12,1)#1.                                                        BOND0580
      W(12,2)#1.                                                        BOND0590
      IF(W(6,1)-W(6,2))165,175,175                                      BOND0600
C     *****VECTOR FROM ATOM TO VIEWPOINT *****                          BOND0610
  152 DO 160 I#1,2                                                      BOND0620
      DO 155 J#10,12                                                    BOND0630
  155 W(J,I)#-W(J-6,I)                                                  BOND0640
      W(12,I)#W(12,I)+VIEW                                              BOND0650
C     ***** DISTANCE SQUARED TO VIEWPOINT *****                         BOND0660
  160 W(13,I)#VV(W(10,I),W(10,I))                                       BOND0670
      IF(W(13,2)-W(13,1))165,175,175                                    BOND0680
C     ***** SWITCH ATOMS *****                                          BOND0690
  165 DO 170 J#1,13                                                     BOND0700
      T1#W(J,1)                                                         BOND0710
      W(J,1)#W(J,2)                                                     BOND0720
  170 W(J,2)#T1                                                         BOND0730
C     ***** FORM IDEMFACTOR MATRIX *****                                BOND0740
  175 DO 180 J#1,3                                                      BOND0750
      E(J,J)#1.                                                         BOND0760
      E(J+1,1)#0.                                                       BOND0770
  180 E(J+5,1)#0.                                                       BOND0780
C     ***** FORM VECTOR SET RADIAL TO BOND *****                        BOND0790
      CALL DIFV(W(4,2),W(4,1),DA(1,3))                                  BOND0800
      CALL UNIT(DA(1,3),V3,1)                                           BOND0810
      T6#ABSF(V3(3))                                                    BOND0820
      IF(.9994-T6)390,185,185                                           BOND0830
  185 T1#CD(3,NB)/SCAL2                                                 BOND0840
      CALL AXES(V3,E(1,3),B,1)                                          BOND0850
      DO 190 J#1,3                                                      BOND0860
      DA(J,1)#-B(J,2)*T1                                                BOND0870
  190 DA(J,2)#-B(J,3)*T1                                                BOND0880
      IF(NBND)500,500,195                                               BOND0890
  195 CALL RADIAL(3)                                                    BOND0900
C     ***** DERIVE QUADRICS FOR EACH ATOM *****                         BOND0910
      DO 380 II#1,2                                                     BOND0920
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      CALL PAXES(W(1,II),2)                                             BOND0930
      IF(NG)205,210,205                                                 BOND0940
  205 CALL ERPNT(W(1,II),800)                                           BOND0950
      GO TO 999                                                         BOND0960
C     ***** DOES BOND GO TO ELLIPSOID OR TO ENVELOPE *****              BOND0970
  210 T1#3-II*2                                                         BOND0980
      DO 212 J#1,3                                                      BOND0990
      V3(J)#V3(J)*T1                                                    BOND1000
  212 VUE(J)#0.                                                         BOND1010
      IF(KD(5,NB))260,260,215                                           BOND1020
  215 CALL UNIT(W(10,II),R(1,3),1)                                      BOND1030
      IF(VMV(V3,Q,R(1,3)))220,260,260                                   BOND1040
C     ***** ESTABLISH VIEW COORDINATE SYSTEM *****                      BOND1050
  220 IBND#0                                                            BOND1060
      IF(VIEW)225,225,230                                               BOND1070
C     ***** DERIVE TANGENT CYLINDER *****                               BOND1080
  225 CONE#0.                                                           BOND1090
      GO TO 240                                                         BOND1100
C     ***** DERIVE TANGENT CONE *****                                   BOND1110
  230 CONE#SCL*SCL/W(13,II)                                             BOND1120
      CALL NORM(E(1,2),R(1,3),R(1,1),1)                                 BOND1130
      CALL UNIT(R(1,1),R(1,1),1)                                        BOND1140
      CALL NORM(R(1,3),R(1,1),R(1,2),1)                                 BOND1150
      DO 235 I#1,3                                                      BOND1160
      DO 235 J#1,3                                                      BOND1170
  235 RT(I,J)#R(J,I)                                                    BOND1180
C     ***** BASE ELLIPSOID ON VIEW COORDINATE SYSTEM *****              BOND1190
      CALL MM(RT,Q,U)                                                   BOND1200
      CALL MM(U,R,Q)                                                    BOND1210
  240 T1#1./(CONE-Q(3,3))                                               BOND1220
      T2#CONE*T1                                                        BOND1230
      DO 250 J#1,2                                                      BOND1240
      DO 245 K#1,2                                                      BOND1250
  245 S(K,J)#Q(K,J)+Q(K,3)*Q(J,3)*T1                                    BOND1260
      S(3,J)#Q(3,J)*T2                                                  BOND1270
  250 S(J,3)#Q(J,3)*T2                                                  BOND1280
      S(3,3)#Q(3,3)*T2                                                  BOND1290
      IF(CONE)252,270,252                                               BOND1300
  252 DO 255 J#1,3                                                      BOND1310
  255 VUE(J)#-W(J+9,II)/SCL                                             BOND1320
C     ***** BASE TANGENT CONE ON WORKING SYSTEM *****                   BOND1330
      CALL MM(R,S,U)                                                    BOND1340
      CALL MM(U,RT,S)                                                   BOND1350
      T5#0.                                                             BOND1360
      GO TO 300                                                         BOND1370
C     ***** TRANSFER ELLIPSOID *****                                    BOND1380
  260 DO 265 J#1,9                                                      BOND1390
  265 S(J,1)#Q(J,1)                                                     BOND1400
      IBND#II                                                           BOND1410
  270 T5#1.                                                             BOND1420
C     ***** CHECK FOR BOND TAPER *****                                  BOND1430
  300 IF(II-2)305,310,310                                               BOND1440
  305 RADIUS#1.+T6*TAPER                                                BOND1450
      GO TO 320                                                         BOND1460
  310 RADIUS#1.-T6*TAPER                                                BOND1470
  320 CALL MV(S,V3,V4)                                                  BOND1480
      T2#VV(V3,V4)                                                      BOND1490
C     ***** COMPUTE BOND INTERSECTION *****                             BOND1500
      KL#5-II-II                                                        BOND1510
      DO 360 K#1,65,4                                                   BOND1520
      DO 325 J#1,3                                                      BOND1530
      V6(J)#D(J,K)*RADIUS                                               BOND1540
  325 V5(J)#V6(J)+VUE(J)                                                BOND1550
      T3#VV(V5,V4)                                                      BOND1560
      T4#T3*T3-T2*(VMV(V5,S,V5)-T5)                                     BOND1570
      IF(T4)330,335,335                                                 BOND1580
  330 NG#13                                                             BOND1590
      CALL ERPNT(W(1,II),800)                                           BOND1600
      GO TO 999                                                         BOND1610
  335 T4#SQRTF(T4)                                                      BOND1620
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      T1#(T4-T3)/T2                                                     BOND1630
      T3#(-T4-T3)/T2                                                    BOND1640
      L#K+KL-1                                                          BOND1650
      DO 360 J#1,3                                                      BOND1660
      D(J,L)#(V6(J)+T1*V3(J))*SCL                                       BOND1670
  360 D(J,L+1)#(-V6(J)-T3*V3(J))*SCL                                    BOND1680
      CALL PRCJ(D(1,KL)  ,DP(1,II),W(4,II),XO,VIEW,1,65,4)              BOND1690
      IF(IBND-1)370,365,370                                             BOND1700
  365 CALL PRCJ(D(1,KL+5),DP(1,II+68),W(4,II),XO,VIEW,1,61,4)           BOND1710
      GO TO 380                                                         BOND1720
C     ***** RETRACE TOP HALF *****                                      BOND1730
  370 DO 375 K#4,64,4                                                   BOND1740
      L#K+II                                                            BOND1750
      M#L+64                                                            BOND1760
      N#66-L                                                            BOND1770
      DP(1,M)#DP(1,N)                                                   BOND1780
  375 DP(2,M)#DP(2,N)                                                   BOND1790
  380 CONTINUE                                                          BOND1800
C     ***** CHECK FOR OVERLAP OR HIDDEN BOND *****                      BOND1810
      DO 395 K#1,65,32                                                  BOND1820
      T1#0.                                                             BOND1830
      T2#0.                                                             BOND1840
      DO 385 J#1,2                                                      BOND1850
      T1#T1+(DP(J,K)-W(J+1,1))**2                                       BOND1860
  385 T2#T2+(DP(J,K+1)-W(J+1,1))**2                                     BOND1870
      IF(T2-T1)390,390,395                                              BOND1880
  390 NG#14                                                             BOND1890
      CALL ERPNT(W(1,2),800)                                            BOND1900
      GO TO 999                                                         BOND1910
  395 CCNTINUE                                                          BOND1920
C     ***** DRAW BCND OUTLINE *****                                     BOND1930
      CALL DRAW(DP(1,1),0.,0.,3)                                        BOND1940
      DO 415 K#5,129,4                                                  BOND1950
  415 CALL DRAW(DP(1,K),0.,0.,2)                                        BOND1960
      DO 420 K#2,66,4                                                   BOND1970
  420 CALL DRAW(DP(1,K),0.,0.,2)                                        BOND1980
      CALL DRAW(DP(1,65),0.,0.,2)                                       BOND1990
C     ***** DRAW BCND DETAIL *****                                      BOND2000
  425 K#65                                                              BOND2010
  430 K#K-NBND                                                          BOND2020
      IF(K-1)500,500,435                                                BOND2030
  435 CALL DRAW(DP(1,K),0.,0.,3)                                        BOND2040
      CALL DRAW(DP(1,K+1),0.,0.,2)                                      BOND2050
      K#K-NBND                                                          BOND2060
      IF(K-1)500,500,440                                                BOND2070
  440 CALL DRAW(DP(1,K+1),0.,0.,3)                                      BOND2080
      CALL DRAW(DP(1,K),0.,0.,2)                                        BOND2090
      GO TO 430                                                         BOND2100
  500 HGT#CD(4,NB)                                                      BOND2110
      OFF#CD(5,NB)                                                      BOND2120
      IF(HGT)510,570,510                                                BOND2130
C     ***** PERSPECTIVE BCND LABEL ROUTINE *****                        BOND2140
C     ***** BASE DECISICNS ON REFERENCE SYSTEM *****                    BOND2150
  510 K#0                                                               BOND2160
      CALL DIFV(W(7,2),W(7,1),V7)                                       BOND2165
      CALL VM(V7,AAREV,V1)                                              BOND2170
      CALL AXES(V1,E(1,3),U,I)                                          BOND2180
      DO 535 I#1,3                                                      BOND2190
      T1#1.                                                             BOND2200
      IF(I-2)515,515,520                                                BOND2210
  515 IF(VV(U(1,I),SYMB(1,I)))525,530,530                               BOND2220
  520 IF(XMODF(K,2))530,525,530                                         BOND2230
  525 T1#-1.                                                            BOND2240
      K#K+1                                                             BOND2250
  530 DO 535 J#1,3                                                      BOND2260
      U(J,I)#U(J,I)*T1                                                  BOND2270
  535 VT(J,I)#B(J,I)*T1                                                 BOND2280
      DO 540 J#1,3                                                      BOND2290
  540 VT(J,4)#.5*(W(J+3,1)+W(J+3,2))                                    BOND2300
C     ***** CHECK FOR EXCESS FORESHORTENING *****                       BOND2310
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      IF(FORE-ABSF(U(3,1)))545,550,550                                  BOND2320
  545 CALL NORM(U(1,2),SYMB(1,3),VT(1,1),1)                             BOND2330
      VT(1,3)#SYMB(1,3)                                                 BOND2340
      VT(2,3)#SYMB(2,3)                                                 BOND2350
      VT(3,3)#SYMB(3,3)                                                 BOND2360
      HGT#CD(6,NB)                                                      BOND2370
      OFF#CD(7,NB)                                                      BOND2380
      IF(HGT)550,999,550                                                BOND2390
  550 TI#CD(8,NB)                                                       BOND2400
      Z(1)#VT(1,4)-HGT*(23.-3.*TI)/7.                                   BOND2410
      Z(2)#VT(2,4)+OFF-HGT*.5                                           BOND2420
      Z(3)#VT(3,4)                                                      BOND2430
      ITILT#1                                                           BOND2440
      IF(TI)555,560,565                                                 BOND2450
  555 CALL NOMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.1)                         BOND2460
      GO TO 570                                                         BOND2470
  560 CALL NOMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.2)                         BOND2480
      GO TO 570                                                         BOND2490
  565 CALL NOMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.3)                         BOND2500
  570 ITILT#0                                                           BOND2510
      IF(NJ2-10)580,999,999                                             BOND2520
  580 WRITE OUTPUT TAPE NOUT,571,DIST                                   BOND2530
  571 FORMAT(1H 59X,10HDISTANCE #F8.3/1H )                              BOND2540
  999 RETURN                                                            BOND2550
      END                                                               BOND2560
*LIST8
*LABEL
      SUBROUTINE DIFV(X,Y,Z)                                            DIFV0010
C     VECTOR - VECTOR                                                   DIFV0020
C     Z(3)#X(3)-Y(3)                                                    DIFV0030
      DIMENSIONX(3),Y(3),Z(3)                                           DIFV0040
      DO111I#1,3                                                        DIFV0050
  111 Z(I)#X(I)-Y(I)                                                    DIFV0060
      RETURN                                                            DIFV0070
      END                                                               DIFV0080
*LIST8
*LABEL
      SUBROUTINE DRAW(W,DX,DY,NPEN)                                     DRAW0010
      DIMENSION W(3),X(3),Y(3),Z(3)                                     DRAW0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    DRAW0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)DRAW0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) DRAW0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) DRAW0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   DRAW0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   DRAW0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     DRAW0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   DRAW0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD DRAW0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIDRAW0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   DRAW0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                DRAW0140
      Y(1)#W(1)+DX                                                      DRAW0150
      Y(2)#W(2)+DY                                                      DRAW0160
      IF(ITILT)115,140,115                                              DRAW0170
C     ***** ROTATE FOR PERSPECTIVE TITLE *****                          DRAW0180
  115 Y(3)#W(3)                                                         DRAW0190
      DO 120 I#1,3                                                      DRAW0200
  120 Z(I)#Y(I)-VT(I,4)                                                 DRAW0210
      DO 130 I#1,3                                                      DRAW0220
  130 X(I)#VT(I,1)*Z(1)+VT(I,2)*Z(2)+VT(I,3)*Z(3)+VT(I,4)               DRAW0230
      CALL PLTXY(X,Y)                                                   DRAW0240
C     ***** CHECK BOUNDRY *****                                         DRAW0250
  140 DO 160 J#1,2                                                      DRAW0260
      IF(Y(J)-XLNG(J)+.1)150,150,145                                    DRAW0270
  145 Y(J)#XLNG(J)-.1                                                   DRAW0280
  150 IF(Y(J)-.1)155,160,160                                            DRAW0290
  155 Y(J)#.1                                                           DRAW0300
  160 CONTINUE                                                          DRAW0310
      CALL PLOT(Y(1),Y(2),NPEN)                                         DRAW0320
      RETURN                                                            DRAW0330
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      END                                                               DRAW0340
*LIST8
*LABEL
      SUBROUTINE EIGEN (W,VALU,VECT)                                    EIGE0010
C     ***** EIGENVALUES AND EIGENVECTORS OF 3X3 MATRIX *****            EIGE0020
      DIMENSION W(3,3),VALU(3),VECT(3,3),A(3,3),B(3,3),V(3),U(3)        EIGE0030
      COMMON NG                                                         EIGE0040
C     ***** STATEMENT FUNCTION *****                                    EIGE0050
      PHIF(Z)#((B2-Z)*Z+B1)*Z+B0                                        EIGE0060
C     ***** START OF PROGRAM *****                                      EIGE0070
      ERRND#5.E-8                                                       EIGE0080
      SIGMA#0.                                                          EIGE0090
      DO 115 J#1,3                                                      EIGE0100
      DO 115 I#1,3                                                      EIGE0110
      TEM#W(I,J)                                                        EIGE0120
      A(I,J)#TEM                                                        EIGE0130
  115 SIGMA#SIGMA+TEM*TEM                                               EIGE0140
C     ***** CHECK FOR NULL MATRIX *****                                 EIGE0150
      IF(SIGMA)230,230,120                                              EIGE0160
  120 SIGMA#SQRTF(SIGMA)                                                EIGE0170
C     ***** FORM CHARACTERISTIC EQUATION *****                          EIGE0180
      B2#A(1,1)+A(2,2)+A(3,3)                                           EIGE0190
      B1#-A(1,1)*A(2,2)-A(1,1)*A(3,3)-A(2,2)*A(3,3)+A(1,3)*A(3,1)       EIGE0200
     1+A(2,3)*A(3,2)+A(1,2)*A(2,1)                                      EIGE0210
      B0#A(1,1)*A(2,2)*A(3,3)+A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(3,2)*A(2,1)-EIGE0220
     1A(1,3)*A(3,1)*A(2,2)-A(1,1)*A(2,3)*A(3,2)-A(1,2)*A(2,1)*A(3,3)    EIGE0230
C     ***** FIRST ROOT BY BISECTION *****                               EIGE0240
      X#0.                                                              EIGE0250
      Y#SIGMA                                                           EIGE0260
      TEM#PHIF(SIGMA)                                                   EIGE0270
      VNEW#0.0                                                          EIGE0280
      IF(B0)135,250,145                                                 EIGE0290
  135 IF(TEM)140,140,165                                                EIGE0300
  140 Y#-Y                                                              EIGE0310
      GO TO 165                                                         EIGE0320
  145 Y#0.                                                              EIGE0330
      X#SIGMA                                                           EIGE0340
      IF(TEM)165,165,150                                                EIGE0350
  150 X#-X                                                              EIGE0360
C     ***** NOW PHIF(X).LT.0.AND.PHIF(Y).GT.0. *****                    EIGE0370
  165 VNEW#(X+Y)*.5                                                     EIGE0380
      DO 225 I#1,40                                                     EIGE0390
  175 IF(PHIF(VNEW))180,250,185                                         EIGE0400
  180 X#VNEW                                                            EIGE0410
      GO TO 200                                                         EIGE0420
  185 Y#VNEW                                                            EIGE0430
  200 VOLD#VNEW                                                         EIGE0440
      VNEW#(X+Y)*.5                                                     EIGE0450
      TEM#ABSF(VOLD-VNEW)                                               EIGE0460
      IF(TEM-ERRND)250,250,205                                          EIGE0470
  205 IF(VOLD)210,225,210                                               EIGE0480
  210 IF(ABSF(TEM/VOLD)-ERRND)250,250,225                               EIGE0490
  225 CONTINUE                                                          EIGE0500
C     ***** DID NOT CONVERGE, SET ERROR INDICATOR *****                 EIGE0510
  230 NG#6                                                              EIGE0520
      GO TO 400                                                         EIGE0530
C     ***** STORE FIRST ROOT *****                                      EIGE0540
  250 U(3)#VNEW                                                         EIGE0550
C     ***** DEFLATE *****                                               EIGE0560
      C1#B2-VNEW                                                        EIGE0570
      C0#B1+C1*VNEW                                                     EIGE0580
C     ***** SOLVE QUADRATIC *****                                       EIGE0590
      TEM#C1*C1+4.*C0                                                   EIGE0600
      IF(TEM)255,265,260                                                EIGE0610
C     ***** IGNORE IMAGINARY COMPONENT OF COMPLEX ROOT *****            EIGE0620
  255 TEM#0.                                                            EIGE0630
      GO TO 265                                                         EIGE0640
  260 TEM#SQRTF(TEM)                                                    EIGE0650
  265 U(1)#.5*(C1-TEM)                                                  EIGE0660
      U(2)#.5*(C1+TEM)                                                  EIGE0670
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C     ***** SORT ROOTS *****                                            EIGE0680
      DO 275 J#1,2                                                      EIGE0690
      IF(U(J)-U(3))275,275,270                                          EIGE0700
  270 TEM#U(J)                                                          EIGE0710
      U(J)#U(3)                                                         EIGE0720
      U(3)#TEM                                                          EIGE0730
  275 CONTINUE                                                          EIGE0740
      LLL#-2                                                            EIGE0750
      DO 375 III#1,2                                                    EIGE0760
C     ***** CHECK FOR MULTIPLE ROOTS *****                              EIGE0770
      TEM#ERRND*100.                                                    EIGE0780
      NG#0                                                              EIGE0790
      L#1                                                               EIGE0800
      DO 305 I#1,2                                                      EIGE0810
      IF(U(I+1)-U(I)-TEM)300,300,290                                    EIGE0820
  290 IF(U(I))295,305,295                                               EIGE0830
  295 IF(ABSF((U(I+1)-U(I))/U(I))-TEM)300,300,305                       EIGE0840
  300 L#L-1                                                             EIGE0850
      NG#NG-2*I                                                         EIGE0860
  305 CONTINUE                                                          EIGE0870
      IF(LLL-L)308,400,400                                              EIGE0880
  308 LLL#L                                                             EIGE0890
C     ***** EIGENVECTOR ROUTINE *****                                   EIGE0900
      DO 375 II#1,3                                                     EIGE0910
      TI#U(II)                                                          EIGE0920
      IF(L)315,310,322                                                  EIGE0930
C     ***** TWO VECTORS NULL FOR DOUBLE ROOT *****                      EIGE0940
  310 IF(NG+5-II)315,322,315                                            EIGE0950
C     ***** ALL VECTORS NULL FOR TRIPLE ROOT *****                      EIGE0960
  315 DO 320 J#1,3                                                      EIGE0970
  320 VECT(J,II)#0.0                                                    EIGE0980
      GO TO 375                                                         EIGE0990
  322 DO 325 J#1,3                                                      EIGE1000
  325 A(J,J)#W(J,J)-TI                                                  EIGE1010
      SMAX#0.0                                                          EIGE1020
      DO 355 I#1,3                                                      EIGE1030
      II#I                                                              EIGE1040
      IF(I-2)335,335,340                                                EIGE1050
  335 II#I+1                                                            EIGE1060
  340 B(I,1)#A(I,2)*A(II,3)-A(I,3)*A(II,2)                              EIGE1070
      B(I,2)#A(I,3)*A(II,1)-A(I,1)*A(II,3)                              EIGE1080
      B(I,3)#A(I,1)*A(II,2)-A(I,2)*A(II,1)                              EIGE1090
      TEM#B(I,1)**2+B(I,2)**2+B(I,3)**2                                 EIGE1100
      IF(TEM-SMAX)355,355,350                                           EIGE1110
  350 SMAX#TEM                                                          EIGE1120
      IMAX#I                                                            EIGE1130
  355 CONTINUE                                                          EIGE1140
      IF(SMAX)353,353,360                                               EIGE1150
  353 NG#7                                                              EIGE1160
      GO TO 375                                                         EIGE1170
  360 SMAX#SQRTF(SMAX)                                                  EIGE1180
      DO 365 J#1,3                                                      EIGE1190
  365 V(J)#B(IMAX,J)/SMAX                                               EIGE1200
C     ***** REFINE EIGENVECTOR *****                                    EIGE1210
      CALL AXEQB(A,V,V,1)                                               EIGE1220
      TEM#MAXIF(ABSF(V(1)),ABSF(V(2)),ABSF(V(3)))                       EIGE1230
      DO 370 J#1,3                                                      EIGE1240
  370 V(J)#V(J)/TEM                                                     EIGE1250
      CALL UNIT(V,VECT(1,II),1)                                         EIGE1260
C     ***** REFINE EIGENVALUE *****                                     EIGE1270
      TI#VMV(VECT(1,II),W,VECT(1,II))                                   EIGE1280
      U(II)#TI                                                          EIGE1290
  375 VALU(II)#TI                                                       EIGE1300
  400 RETURN                                                            EIGE1310
      END                                                               EIGE1320
*LIST8
*LABEL
      SUBROUTINE ERPNT(TI,N)                                            ERPN0010
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ERPN0020
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)ERPN0030
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      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) ERPN0040
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ERPN0050
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   ERPN0060
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ERPN0070
      DIMENSION XLNG(3),XO(3),XT(3)                                     ERPN0080
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ERPN0090
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ERPN0100
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIERPN0110
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ERPN0120
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ERPN0130
      WRITE OUTPUT TAPE NOUT,115,NG,TI,N                                ERPN0140
  115 FORMAT(1H 10X,10HFAULT NG #I3,F10.0,I6/1H )                       ERPN0150
      NG#0                                                              ERPN0160
      RETURN                                                            ERPN0170
      END                                                               ERPN0180
*LIST8
*LABEL
      SUBROUTINE F200                                                   F2000010
      DIMENSION PLA(2000)                                               F2000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F2000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F2000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F2000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F2000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F2000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F2000080
      DIMENSION XLNG(3),XO(3),XT(3)                                     F2000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F2000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F2000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF2000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F2000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F2000140
C     ***** CALCOMP CONTROL *****                                       F2000150
      IF(NJ2-1)216,210,212                                              F2000160
  210 CALL PLOTS(PLA(2000),1998,LTNO)                                   F2000170
C     ***** FOR CDC 1604 A USE  210 CALL PLOTS(PLA,2000,LTNO)   *****   F2000175
C     ***** FOR IBM 7090 USE  210 CALL PLOTS(PLA(2000),1998,LTNO)  *****F2000176
      GO TO 216                                                         F2000180
  212 CALL PLOT(AIN(1),AIN(2),-3)                                       F2000190
  216 RETURN                                                            F2000200
      END                                                               F2000210
*LIST8
*LABEL
      SUBROUTINE F400                                                   F4000010
C     ***** ATOM LIST FUNCTIONS *****                                   F4000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F4000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F4000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F4000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F4000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F4000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F4000080
      DIMENSION XLNG(3),XO(3),XT(3)                                     F4000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F4000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F4000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF4000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F4000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F4000140
      NG#0                                                              F4000150
      IF(LATM)402,402,400                                               F4000160
  400 DO 401 I#1,LATM                                                   F4000170
  401 CALL ATOM(ATOMS(1,I),ATOMS(2,I))                                  F4000180
  402 IF(XMODF(NJ2,10)-1)499,404,403                                    F4000190
  403 CALL SEARCH                                                       F4000200
      GO TO 499                                                         F4000210
C     ***** STORES (401) OR REMOVES (411) RUNS OF ATOMS *****           F4000220
C     ***** RUN HIERARCHY # ATOM NO./SYM/ A/B/C TRANS. *****            F4000230
  404 II#1                                                              F4000240
C     ***** FIND RUNS IN AIN ARRAY *****                                F4000250
  405 TI#AIN(II)                                                        F4000260
      IF(TI)410,410,420                                                 F4000270
  410 II#II+1                                                           F4000280
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      IF(140-II)499,405,405                                             F4000290
  420 JJ#II                                                             F4000300
C     ***** SET INITIAL RUN VALUES *****                                F4000310
      M1#T1/100000.                                                     F4000320
      M2#MODF(T1,100.)                                                  F4000330
      M5#MODF(T1/100.,1000.)                                            F4000340
      IF(M5)422,422,423                                                 F4000350
  422 M5#555                                                            F4000360
  423 M3#M5/100                                                         F4000370
      M4#XMODF(M5/10,10)                                                F4000380
      M5#XMODF(M5,10)                                                   F4000390
  425 JJ#JJ+1                                                           F4000400
      IF(140-JJ)435,430,430                                             F4000410
  430 T2#-AIN(JJ)                                                       F4000420
      IF(T2)435,425,440                                                 F4000430
  435 II#JJ-1                                                           F4000440
C     ***** SET TERMINAL VALUES FOR DEGENERATE RUN *****                F4000450
      N1#M1                                                             F4000460
      N2#M2                                                             F4000470
      N3#M3                                                             F4000480
      N4#M4                                                             F4000490
      N5#M5                                                             F4000500
      GO TO 450                                                         F4000510
  440 II#JJ                                                             F4000520
C     ***** SET TERMINAL RUN VALUES *****                               F4000530
      N1#T2/100000.                                                     F4000540
      N2#MODF(T2,100.)                                                  F4000550
      N5#MODF(T2/100.,1000.)                                            F4000560
      IF(N5)445,445,446                                                 F4000570
  445 N5#555                                                            F4000580
  446 N3#N5/100                                                         F4000590
      N4#XMODF(N5/10,10)                                                F4000600
      N5#XMODF(N5,10)                                                   F4000610
C     ***** LOOP THROUGH ALL RUNS *****                                 F4000620
  450 DO 490 L5#M5,N5                                                   F4000630
      DO 490 L4#M4,N4                                                   F4000640
      DO 490 L3#M3,N3                                                   F4000650
      DO 490 L2#M2,N2                                                   F4000660
      DO 490 L1#M1,N1                                                   F4000670
      V1(1)#FLOATF(L1)*100000.+FLOATF(L3*10000+L4*1000+L5*100+L2)       F4000680
      CALL ATOM(V1(1),V1(2))                                            F4000690
      IF(NG)455,458,455                                                 F4000700
  455 CALL ERPNT(V1(1),401)                                             F4000710
      GO TO 490                                                         F4000720
  458 CALL STORE                                                        F4000730
  490 CONTINUE                                                          F4000740
      GO TO 410                                                         F4000750
  499 RETURN                                                            F4000760
      END                                                               F4000770
*LIST8
*LABEL
      SUBROUTINE F500                                                   F5000010
      DIMENSION RM(3,3),V(3,4)                                          F5000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F5000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F5000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F5000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F5000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F5000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F5000080
      DIMENSION XLNG(3),XO(3),XT(3)                                     F5000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F5000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F5000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF5000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F5000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F5000140
      NG#0                                                              F5000150
      IF(NJ2-1)599,501,510                                              F5000160
  501 T1#AIN(1)                                                         F5000170
      CALL ATOM(T1,ORGN)                                                F5000180
      IF(NG)502,504,502                                                 F5000190
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  502 CALL ERPNT(TI,501)                                                F5000200
      CALL EXIT                                                         F5000210
  504 DO 506 K#1,4                                                      F5000220
      TI#AIN(K+1)                                                       F5000230
      CALL ATCM(TI,V(1,K))                                              F5000240
      IF(NG)502,506,502                                                 F5000250
  506 CONTINUE                                                          F5000260
      DO 507 J#1,3                                                      F5000270
      V1(J)#V(J,2)-V(J,1)                                               F5000280
  507 V2(J)#V(J,4)-V(J,3)                                               F5000290
      IND#-1                                                            F5000300
      IF(AIN(7))509,509,508                                             F5000310
  508 IND#-2                                                            F5000320
  509 CALL AXES(V1,V2,REFV,IND)                                         F5000330
      GO TO 562                                                         F5000340
  510 DO 552 L#1,139,2                                                  F5000350
      I#AIN(L)                                                          F5000360
      IF(I)532,552,512                                                  F5000370
  512 X#AIN(L+1)*0.01745329252                                          F5000380
      T1#COSF(X)                                                        F5000390
      T2#SINF(X)                                                        F5000400
      I3#XMODF(I+2,3)+1                                                 F5000410
      I1#XMODF(I3,3)+1                                                  F5000420
      I2#XMODF(I1,3)+1                                                  F5000430
      RM(I1,I1)#T1                                                      F5000440
      RM(I1,I2)#T2                                                      F5000450
      RM(I1,I3)#0.0                                                     F5000460
      RM(I2,I1)#-T2                                                     F5000470
      RM(I2,I2)#T1                                                      F5000480
      RM(I2,I3)#0.0                                                     F5000490
      RM(I3,I1)#0.0                                                     F5000500
      RM(I3,I2)#0.0                                                     F5000510
      RM(I3,I3)#1.0                                                     F5000520
      CALL MM(REFV,RM,V)                                                F5000530
      IF(NJ2-3)518,525,599                                              F5000540
  518 DO 522 J#1,9                                                      F5000550
  522 REFV(J,1)#V(J,1)                                                  F5000560
      GO TO 552                                                         F5000570
  525 DO 528 J#1,9                                                      F5000580
  528 WRKV(J,1)#V(J,1)                                                  F5000590
      GO TO 552                                                         F5000600
  532 IF(NJ2-3)535,552,599                                              F5000610
  535 I#XMODF(-I,3)                                                     F5000620
      DO 542 J#1,I                                                      F5000630
      DO 542 K#1,3                                                      F5000640
      T1#REFV(K,3)                                                      F5000650
      REFV(K,3)#REFV(K,2)                                               F5000660
      REFV(K,2)#REFV(K,1)                                               F5000670
  542 REFV(K,1)#T1                                                      F5000680
  552 CONTINUE                                                          F5000690
      IF(NJ2-3)562,582,599                                              F5000700
  562 CALL MM(AA,REFV,AAREV)                                            F5000710
      DO 572 J#1,9                                                      F5000720
      WRKV(J,1)#REFV(J,1)                                               F5000730
  572 AAWRK(J,1)#AAREV(J,1)                                             F5000740
      GO TO 599                                                         F5000750
  582 CALL MM(AA,WRKV,AAWRK)                                            F5000760
  599 RETURN                                                            F5000770
      END                                                               F5000780
*LIST8
*LABEL
      SUBROUTINE F600                                                   F6000010
C     ***** SCALING AND CENTERING FUNCTIONS *****                       F6000020
      DIMENSION MAX(3),SCAL(4),X(3),XMAX(3),XMIN(3),Z(2)                F6000030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F6000040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F6000050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F6000060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F6000070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F6000080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F6000090
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      DIMENSION XLNG(3),XO(3),XT(3)                                     F6000100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F6000110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F6000120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF6000130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2   F6000140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F6000150
C     ***** DEL # 1. FOR INCRUMENTING FUNCTIONS *****                   F6000160
C     ***** DEL # 0. FOR REGULAR FUNCTIONS *****                        F6000170
      DEL#FLOATF(XMODF(NJ2/10,2))                                       F6000180
      NJ2#XMODF(NJ2,10)                                                 F6000190
C     ***** EXPLICIT ORIGIN AND SCALE *****                             F6000200
      IF(AIN(1))602,604,602                                             F6000210
  602 XO(1)#AIN(1)+XO(1)*DEL                                            F6000220
  604 IF(AIN(2))606,608,606                                             F6000230
  606 XO(2)#AIN(2)+XO(2)*DEL                                            F6000240
  608 IF(AIN(3))612,612,609                                             F6000250
  609 IF(DEL)611,611,610                                                F6000260
  610 SCAL1#SCAL1*AIN(3)                                                F6000270
      GO TO 612                                                         F6000280
  611 SCAL1#AIN(3)                                                      F6000290
  612 IF(AIN(4))616,616,614                                             F6000300
C     ***** SET ELLIPSOID SCALE FACTOR *****                            F6000310
  614 SCAL2#AIN(4)                                                      F6000320
C     ***** AUTOMATIC ORIGIN AND/OR SCALE *****                         F6000330
  616 IF(NJ2-2)790,622,620                                              F6000340
  620 XO(1)#XLNG(1)*.5                                                  F6000350
      XO(2)#XLNG(2)*.5                                                  F6000360
  622 IF(NJ2-3)625,640,625                                              F6000370
  625 SCAL1#1.                                                          F6000380
  630 IF(LATM-1)635,635,640                                             F6000390
  635 NG#12                                                             F6000400
      CALL ERPNT(0.,602)                                                F6000410
      CALL EXIT                                                         F6000420
  640 DO 650 J#1,3                                                      F6000430
      XMAX(J)#-1.E5                                                     F6000440
  650 XMIN(J)#1.E5                                                      F6000450
C     ***** FIT BOX AROUND SET OF ATOMS *****                           F6000460
      DO 670 I#1,LATM                                                   F6000470
      CALL XYZ(ATOMS(1,I),ATOMS(2,I),3)                                 F6000480
      IF(NG)652,653,652                                                 F6000490
  652 CALL ERPNT(ATOMS(1,I),600)                                        F6000500
      GO TO 670                                                         F6000510
  653 DO 668 J#1,3                                                      F6000520
      TI#ATOMS(J+1,I)                                                   F6000530
      IF(XMAX(J)-TI)655,660,660                                         F6000540
  655 XMAX(J)#TI                                                        F6000550
      MAX(J)#I                                                          F6000560
  660 IF(TI-XMIN(J))665,668,668                                         F6000570
  665 XMIN(J)#TI                                                        F6000580
  668 CONTINUE                                                          F6000590
  670 CONTINUE                                                          F6000600
C     ***** KM#TOP ATOM *****                                           F6000610
      KM#MAX(3)                                                         F6000620
      SMULT#1.                                                          F6000630
      DO 780 M#1,5                                                      F6000640
      IF(M-2)740,675,678                                                F6000650
C     ***** CHECK VIEW DISTANCE *****                                   F6000660
  675 IF(VIEW)785,785,680                                               F6000670
  678 IF(NJ2-3)680,785,680                                              F6000680
  680 TI#ATOMS(4,KM)*SMULT                                              F6000690
      IF(VIEW*.5-TI)685,690,690                                         F6000700
C     ***** INCREASE VIEW DISTANCE *****                                F6000710
  685 VIEW#2.*TI                                                        F6000720
C     ***** FIND PERSPECTIVE PROJECTION LIMITS *****                    F6000730
  690 DO 700 J#1,2                                                      F6000740
      XMAX(J)#-1.E5                                                     F6000750
  700 XMIN(J)#1.E5                                                      F6000760
      DO 725 I#1,LATM                                                   F6000770
      DO 705 J#1,3                                                      F6000780
  705 X(J)#ATOMS(J+1.I)*SMULT                                           F6000790
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      T2#VIEW/(VIEW-X(3))                                               F6000800
      DO 725 J#1,2                                                      F6000810
      T1#X(J)*T2                                                        F6000820
      IF(XMAX(J)-T1)710,715,715                                         F6000830
  710 XMAX(J)#T1                                                        F6000840
  715 IF(T1-XMIN(J))720,725,725                                         F6000850
  720 XMIN(J)#T1                                                        F6000860
  725 CONTINUE                                                          F6000870
C     ***** REFINE PARAMETERS *****                                     F6000880
  740 IF(NJ2 -3)745,742,755                                             F6000890
  742 SMUL2#1.                                                          F6000900
      GO TO 765                                                         F6000910
C     ***** AUTOMATIC SCALE ONLY *****                                  F6000920
  745 DO 750 J#1,2                                                      F6000930
      T2#XO(J)                                                          F6000940
      SCAL(J)#(BRDR-T2)/XMIN(J)                                         F6000950
  750 SCAL(J+2)#(XLNG(J)-BRDR-T2)/XMAX(J)                               F6000960
      SMUL2#MIN1F(SCAL(1),SCAL(2),SCAL(3),SCAL(4))                      F6000970
      GO TO 780                                                         F6000980
C     ***** AUTOMATIC SCALE AND POSITION *****                          F6000990
  755 DO 760 J#1,2                                                      F6001000
  760 SCAL(J)#(XLNG(J)-BRDR*2.)/(XMAX(J)-XMIN(J))                       F6001010
      SMUL2#MIN1F(SCAL(1),SCAL(2))                                      F6001020
C     ***** AUTOMATIC POSITION *****                                    F6001030
  765 DO 770 J#1,2                                                      F6001040
  770 XO(J)#.5*(XLNG(J)-SMUL2*(XMAX(J)+XMIN(J)))                        F6001050
  780 SMULT#SMULT*SMUL2                                                 F6001060
      VIEW#VIEW*SMUL2                                                   F6001070
  785 SCAL1#SCAL1*SMULT                                                 F6001080
  790 SCL#SCAL1*SCAL2                                                   F6001090
      RETURN                                                            F6001100
      END                                                               F6001110
*LIST8
*LABEL
      SUBROUTINE F700                                                   F7000010
C     ***** SUBROUTINE TO DRAW ELLIPSOIDS *****                         F7000020
      DIMENSION EYE(3),VIEWV(3),X(3),Z(3)                               F7000030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F7000040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F7000050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F7000060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F7000070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F7000080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F7000090
      DIMENSION XLNG(3),XO(3),XT(3)                                     F7000100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F7000110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F7000120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F7000130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F7000140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F7000150
C     ***** SET ELLIPSOID GRAPHIC DETAILS *****                         F7000160
      ITILT#0                                                           F7000170
      NG#0                                                              F7000180
      NFIRST#1                                                          F7000190
      NPLANE#AIN(1)                                                     F7000200
      IF(NPLANE-1)720,715,720                                           F7000210
  715 NFIRST#4                                                          F7000220
      NPLANE#4                                                          F7000230
  720 NSOLID#AIN(2)                                                     F7000240
      NDCT#64/2**(XABSF(NSOLID))                                        F7000250
      LINES#AIN(3)                                                      F7000260
      NDASH#AIN(4)                                                      F7000270
      CHSYM#AIN(5)                                                      F7000280
      DH#AIN(6)-CHSYM*17./7.                                            F7000290
      DV#AIN(7)-CHSYM*.5                                                F7000300
C     ***** ESTABLISH REFERENCE POINT OF VIEW *****                     F7000310
      T1#1.E6                                                           F7000320
      IF(VIEW)740,740,735                                               F7000330
  735 T1#VIEW/SCAL1                                                     F7000340
  740 DO 745 J#1,3                                                      F7000350
  745 EYE(J)#REFV(J,3)*T1+ORGN(J)                                       F7000360
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      LNS#-1                                                            F7000370
C     ***** LOOP THROUGH ATOM LIST *****                                F7000380
      DO 1105 ITOM#1,LATM                                               F7000390
      TI#ATOMS(I,ITOM)                                                  F7000400
      CALL XYZ(TI,X,2)                                                  F7000410
      IF(NG)758,746,758                                                 F7000420
  746 CALL PLTXY(X,Z)                                                   F7000430
      K#TI/100000.                                                      F7000440
      L#TI-FLOATF(K)*100000.                                            F7000450
      IF(NJ2-10)747,754,754                                             F7000460
  747 LNS#XMODF(LNS+1,18)                                               F7000470
      IF(LNS)749,748,749                                                F7000480
  748 WRITE OUTPUT TAPE NOUT,751,(TITLE(I),I#1,12)                      F7000490
      WRITE OUTPUT TAPE NOUT,752                                        F7000500
  749 WRITE OUTPUT TAPE NOUT,750,CHEM(K),K,L,Z(1),Z(2),(X(I),I#1,3),(XT(F7000510
     II),I#1,3)                                                         F7000520
  750 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)   2F8.2,3X,3F8.3,11X,3F8.4)    F7000530
  751 FORMAT(1H11 0X,12A6)                                              F7000540
  752 FORMAT(1H31 0X,18HSYMBOL   ATOM CODE7X,16HPLOTTER X,Y(IN.) 3X,21HCAF7000550
     1RTESIAN X,Y,Z (IN.)15X,20HCRYSTAL SYSTEM X,Y,Z/1H 19X,45H(DIRECTIOF7000560
     2N COSINES(I,J),I#1,3),RMSD(J)),J#1,312X,42HFOR PRINCIPAL AXES BASEF7000570
     3D CN WORKING SYSTEM/1H )                                          F7000580
  754 IF(EDGE-BRDR*.75)755,760,760                                      F7000590
  755 NG#10                                                             F7000600
  758 CALL ERPNT(TI,700)                                                F7000610
      GO TO 1105                                                        F7000620
  760 IF(CHSYM)775,775,765                                              F7000630
C     ***** PLOT CHEMICAL SYMBOLS *****                                 F7000640
  765 T4#1.                                                             F7000650
      IF(VIEW)767,767,766                                               F7000660
  766 T4#VIEW/(VIEW-X(3))                                               F7000670
  767 T3#CHSYM*T4                                                       F7000680
      T4#DISP*T4*.5                                                     F7000690
      V1(1)#X(1)+DH*SYMB(1,1)+DV*SYMB(1,2)                              F7000700
      V1(2)#X(2)+DH*SYMB(2,1)+DV*SYMB(2,2)                              F7000710
      V1(3)#X(3)                                                        F7000720
      CALL PLTXY(V1,V3)                                                 F7000730
      IF(EDGE-CHSYM)775,768,768                                         F7000740
  768 V2(3)#0.                                                          F7000750
      DO 770 I#1,3,2                                                    F7000760
      V2(1)#V3(1)+FLOATF(I-2)*T4                                        F7000770
      DO 770 J#1,3,2                                                    F7000780
      V2(2)#V3(2)+FLOATF(J-2)*T4                                        F7000790
      CALL SIMBOL(V2(1),V2(2),T3,CHEM(K),THETA,6)                       F7000800
      IF(T4)775,775,770                                                 F7000810
  770 CONTINUE                                                          F7000820
  775 IF(NPLANE)1105,1105,780                                           F7000830
C     ***** ELLIPSOID PRINC VECTORS TOWARD VIEWER *****                 F7000840
  780 CALL PAXES(TI,2)                                                  F7000850
      IF(NG)758,783,758                                                 F7000860
  783 CALL DIFV(EYE,XT,VIEWV)                                           F7000870
      CALL UNIT(VIEWV,VIEWV,-1)                                         F7000880
      CALL VM(VIEWV,AA,V2)                                              F7000890
      DO 795 I#1,3                                                      F7000900
      IF(VV(V2,PAT(1,I)))785,795,795                                    F7000910
  785 DO 790 J#1,3                                                      F7000920
      PAC(J,I)#-PAC(J,I)                                                F7000930
  790 PAT(J,I)#-PAT(J,I)                                                F7000940
  795 CONTINUE                                                          F7000950
      DO 800 J#1,3                                                      F7000960
      PAC(J,4)#PAC(J,1)                                                 F7000970
  800 PAC(J,5)#PAC(J,2)                                                 F7000980
      IF(NJ2-10)802,803,803                                             F7000990
  801 FORMAT(1H 13X,3(3X,3F8.4,F8.5)/1H )                               F7001000
  802 WRITE OUTPUT TAPE NOUT,801,(((PAC(J,K),J#1,3),RMS(K)),K#1,3)      F7001010
C     ***** V4 # VECTOR NORMAL TO POLAR PLANE *****                     F7001020
  803 CALL VM(VIEWV,AAWRK,V6)                                           F7001030
      CALL UNIT(V6,V6,1)                                                F7001040
      CALL MV(Q,V6,V4)                                                  F7001050
      CALL UNIT(V4,V4,1)                                                F7001060
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C     ***** SET PLOTTING RESOLUTION FOR ELLIPSOID *****                F7001070
      T3#RMS(3)*SCL                                                    F7001080
      NRESOL#1                                                         F7001090
      NBIS#5                                                           F7001100
      DO 805 J#1,3                                                     F7001110
      IF(T3-RES(J))804,810,810                                         F7001120
  804 NBIS#NBIS-1                                                      F7001130
  805 NRESOL#NRESOL*2                                                  F7001140
  810 NRES1#NRESOL+1                                                   F7001150
C     ***** LOOP THROUGH PRINC AND POLAR PLANES *****                  F7001160
      DO 1100 II#NFIRST,NPLANE                                         F7001170
      II0#XMODF(II+2,3)+1                                              F7001180
      III#XMODF(II,3)+1                                                F7001190
      II2#XMODF(II+1,3)+1                                              F7001200
C     ***** GENERATE CONJUGATE DIAMETERS *****                         F7001210
      IF(.99938-ABSF(VV(V4,PAC(1,II2))))820,820,830                    F7001220
  820 T1#RMS(II0)*SCL                                                  F7001230
      T2#RMS(III)*SCL                                                  F7001240
      DO 825 J#1,3                                                     F7001250
      DA(J,1)#PAC(J,II0)*T1                                            F7001260
  825 DA(J,2)#PAC(J,III)*T2                                            F7001270
      GO TO 850                                                        F7001280
  830 CALL NORM(PAC(1,II0),PAC(1,III),V1,1)                            F7001290
      CALL NORM(V1,V4,V2,1)                                            F7001300
      CALL UNIT(V2,V2,1)                                               F7001310
      CALL MV(Q,V2,V3)                                                 F7001320
      IF(II-4)835,840,840                                              F7001330
  835 CALL NORM(V3,V1,V5,1)                                            F7001340
      GO TO 843                                                        F7001350
  840 CALL NORM(V3,V4,V5,1)                                            F7001360
  843 CALL UNIT(V5,V5,1)                                               F7001370
      T1#SCL/SQRTF(VMV(V2,Q,V2))                                       F7001380
      T2#SCL/SQRTF(VMV(V5,Q,V5))                                       F7001390
      DO 845 J#1,3                                                     F7001400
      DA(J,1)#V2(J)*T1                                                 F7001410
  845 DA(J,2)#V5(J)*T2                                                 F7001420
C     ***** GENERATE ELLIPSE *****                                     F7001430
  850 CALL RADIAL(NBIS)                                                F7001440
      IF(II-4)900,855,855                                              F7001450
C     ***** PLOT BOUNDARY ELLIPSE *****                                F7001460
  855 CALL PROJ(D,DP,X,X0,VIEW,1,129,NRESOL)                           F7001470
      CALL DRAW(DP,0.,0.,3)                                            F7001480
      DO 860 J#NRES1,129,NRESOL                                        F7001490
  860 CALL DRAW(DP(1,J),0.,0.,2)                                       F7001500
      IF(DISP)1100,1100,865                                            F7001510
C     ***** BOUNDARY ANNULUS AS A LINEAR FUNCTION OF HEIGHT *****      F7001520
  865 CALL DIFV(XT,ORGN,V1)                                            F7001530
      T5#VV(V1,AAREV(1,3))*SCAL1                                       F7001540
      NCYCLE#.5+(AIN(8)+T5*AIN(9))/DISP                                F7001550
      IF(NCYCLE)1100,1100,870                                          F7001560
  870 T3#(2.*DISP)/(T1+T2)                                             F7001570
C     ***** INCREASE ANNULAR THICKNESS *****                           F7001580
      DO 875 I#1,NCYCLE                                                F7001590
      T4#T3*FLOATF(I)                                                  F7001600
      DO 875 J#1,129,NRESOL                                            F7001610
  875 CALL DRAW(DP(1,J),D(1,J)*T4,D(2,J)*T4,2)                         F7001620
      GO TO 1100                                                       F7001630
  900 CALL PROJ(D,DP,X,X0,VIEW,1,65,NRESOL)                            F7001640
C     ***** PLOT HALF AN ELLIPSE *****                                 F7001650
      CALL DRAW(DP,0.,0.,3)                                            F7001660
      DO 905 J#NRES1,65,NRESOL                                         F7001670
  905 CALL DRAW(DP(1,J),0.,0.,2)                                       F7001680
      IF(DISP)930,930,910                                              F7001690
C     ***** ACCENTUATE FRONT HALF *****                                F7001700
  910 DO 925 I#1,3,2                                                   F7001710
      T2#FLOATF(I-2)*DISP                                              F7001720
      DO 915 J#1,65,NRESOL                                             F7001730
      K#66-J                                                           F7001740
  915 CALL DRAW(DP(1,K),DISP,T2,2)                                     F7001750
      DO 925 K#1,65,NRESOL                                             F7001760
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  925 CALL DRAW(DP(1,K),-DISP,-T2,2)                                    F7001770
  930 IF(NSOLID)940,967,935                                             F7001780
  935 L#NDOT                                                            F7001790
      IF(NDOT-NRESOL)938,945,940                                        F7001800
  938 CALL RADIAL(NSOLID-1)                                             F7001810
      GO TO 945                                                         F7001820
  940 L#NRESOL                                                          F7001830
  945 CALL PROJ(D(1,65),DP(1,65),X,XO,VIEW,1,65,L)                      F7001840
      IF(NSOLID)960,967,950                                             F7001850
C     ***** DOTTED LINE ON REVERSE SIDE *****                           F7001860
  950 DO 958 J#65,129,NDOT                                              F7001870
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    F7001880
      DO 955 I#1,3,2                                                    F7001890
      T1#FLOATF(I-2)*DISP                                               F7001900
      DO 955 K#1,3,2                                                    F7001910
      T2#FLOATF(K-2)*DISP                                               F7001920
      CALL DRAW(DP(1,J),T1,T2,2)                                        F7001930
      IF(DISP)958,958,955                                               F7001940
  955 CONTINUE                                                          F7001950
  958 CONTINUE                                                          F7001960
      GO TO 967                                                         F7001970
C     ***** SINGLE LINE ON REVERSE SIDE *****                           F7001980
  960 DO 965 J#65,129,NRESOL                                            F7001990
  965 CALL DRAW(DP(1,J),0.,0.,2)                                        F7002000
C     ***** DETAIL INTERIOR FEATURES *****                              F7002010
  967 T2#NDASH*2                                                        F7002020
      DO 975 J#1,3                                                      F7002030
      T1#PAC(J,110)*RMS(110)*SCL                                        F7002040
      DA(J,1)#T1                                                        F7002050
      DA(J,2)#PAC(J,111)*RMS(111)*SCL                                   F7002060
      DA(J,3)#0.                                                        F7002070
      IF(NDASH)975,975,970                                              F7002080
  970 V1(J)#-T1                                                         F7002090
      V2(J)#T1/T2                                                       F7002100
  975 CONTINUE                                                          F7002110
      IF(NDASH)987,987,980                                              F7002120
C     ***** DASHED LINE FOR REVERSE AXIS *****                          F7002130
  980 DO 985 J#1,NDASH                                                  F7002140
      DO 985 K#1,2                                                      F7002150
      L#4-K                                                             F7002160
      CALL PROJ(V1,DP,X,XO,VIEW,1,1,1)                                  F7002170
      CALL DRAW(DP,0.,0.,L)                                             F7002180
      DO 985 I#1,3                                                      F7002190
  985 V1(I)#V1(I)+V2(I)                                                 F7002200
C     ***** SOLID LINE FOR FORWARD AXIS *****                           F7002210
  987 IF(LINES)1100,1100,988                                            F7002220
  988 CALL PROJ(DA,DP,X,XO,VIEW,1,3,1)                                  F7002230
      T1#DISP*.5                                                        F7002240
      DO 990 I#1,3,2                                                    F7002250
      T2#FLOATF(2-I)*T1                                                 F7002260
      CALL DRAW(DP,T1,T2,3)                                             F7002270
      CALL DRAW(DP(1,3),T1,T2,2)                                        F7002280
      IF(DISP)1000,1000,989                                             F7002290
  989 CALL DRAW(DP(1,3),-T1,T2,2)                                       F7002300
  990 CALL DRAW(DP,-T1,T2,2)                                            F7002310
C     ***** SHADE QUADRANT BETWEEN TWO PRINCIPAL AXES *****             F7002320
 1000 L#LINES-1                                                         F7002330
      IF(L)1100,1100,1005                                               F7002340
 1005 T2#LINES                                                          F7002350
      DO 1025 I#1,L                                                     F7002360
      T1#FLOATF(I)/T2                                                   F7002370
      T3#SQRTF(1.-T1*T1)                                                F7002380
      IF(XMODF(I,2))1010,1015,1010                                      F7002390
 1010 M#I*2                                                             F7002400
      N#M-1                                                             F7002410
      GO TO 1020                                                        F7002420
 1015 N#I*2                                                             F7002430
      M#N-1                                                             F7002440
 1020 DO 1025 J#1,3                                                     F7002450
      T4#DA(J,1)*T1                                                     F7002460
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      D(J,M)#T4                                                         F7002470
 1025 D(J,N)#DA(J,2)*T3+T4                                              F7002480
      L#L*2                                                             F7002490
      CALL PRCJ(D,DP,X,XO,VIEW,1,L,1)                                   F7002500
      DO 1030 I#2,L,2                                                   F7002510
      CALL DRAW(DP(1,I-1),0.,0.,3)                                      F7002520
 1030 CALL DRAW(DP(1,I),0.,0.,2)                                        F7002530
 1100 CONTINUE                                                          F7002540
 1105 CONTINUE                                                          F7002550
      RETURN                                                            F7002560
      END                                                               F7002570
*LIST8
*LABEL
      SUBROUTINE F800                                                   F8000010
C     ***** SUBROUTINE FINDS ATOM PAIRS FOR BONDS *****                 F8000020
      DIMENSION IA(3),WI(3)                                             F8000030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F8000040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F8000050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F8000060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F8000070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F8000080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F8000090
      DIMENSION XLNG(3),XO(3),XT(3)                                     F8000100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F8000110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F8000120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF8000130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F8000140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F8000150
      LNS#-4                                                            F8000160
      IF(XMODF(NJ2,10)-2)805,840,840                                    F8000170
C     ***** EXPLICIT DESCRIPTION *****                                  F8000180
  805 II#0                                                              F8000190
      IF(NCD)845,845,815                                                F8000200
  815 II#II+1                                                           F8000210
      IF(140-II)899,899,820                                             F8000220
  820 T1#AIN(II)                                                        F8000230
      IF(T1)815,815,825                                                 F8000240
  825 II#II+1                                                           F8000250
      T2#AIN(II)                                                        F8000260
      IF(T2)815,815,830                                                 F8000270
  830 IF(NJ2-10)832,838,838                                             F8000280
  832 LNS#XMODF(LNS+4,56)                                               F8000290
      IF(LNS)838,834,838                                                F8000300
  834 WRITE OUTPUT TAPE NOUT,835,(TITLE(I),I#1,12)                      F8000310
  835 FORMAT(1H110X,12A6)                                               F8000320
      WRITE OUTPUT TAPE NOUT,837                                        F8000330
  837 FORMAT(1H010X,18HSYMBOL   ATOM CODE6X,16HPLOTTER X,Y(IN.) 6X,21HCAF8000340
     1RTESIAN X,Y,Z (IN.)17X,20HCRYSTAL SYSTEM X,Y,Z/1H )               F8000350
  838 CALL BOND(T1,T2,1)                                                F8000360
      GO TO 815                                                         F8000370
C     ***** IMPLICIT DESCRIPTION *****                                  F8000380
  840 IF(LATM-2)845,850,850                                             F8000390
  845 NG#11                                                             F8000400
      CALL ERPNT(0.,NJ*100+NJ2)                                         F8000410
      GO TO 899                                                         F8000420
  850 SCAL3#SCAL1                                                       F8000430
      SCAL1#1.                                                          F8000440
      DO 855 I#1,LATM                                                   F8000450
  855 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                 F8000460
      SCAL1#SCAL3                                                       F8000470
      IF(NCD)845,845,860                                                F8000480
  860 WRITE OUTPUT TAPE NOUT,861                                        F8000490
  861 FORMAT(1H010X,20HBOND SELECTION CODES//11X,94H(SEQUENCE(A))(SEQUENF8000500
     1CE(B)) (BCND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(F8000510
     2DIGITS) /11X,93H(  MIN   MAX )(  MIN   MAX ) (TYPE) (MIN   MAX)(RADIF8000520
     3US)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER))                      F8000530
      DMAX#0.                                                           F8000540
      DO 870 I#1,NCD                                                    F8000550
      IF(DMAX-CD(2,I))865,870,870                                       F8000560
  865 DMAX#CD(2,I)                                                      F8000570
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  870 WRITE OUTPUT TAPE NOUT,871,(KD(J,I),J#1,5),(CD(J,I),J#1,8)          F8000580
  871 FORMAT(1H 10X16,I5,I8,I5,I8,2F6.2,5F8.3,F7.0)                       F8000590
      DMAX#DMAX*DMAX                                                      F8000600
C     ***** LOOP THROUGH ATOMS ARRAY *****                                F8000610
      DO 895 M#1,LATM                                                     F8000620
      T1#ATOMS(1,M)                                                       F8000630
      IA(1)#T1/100000.                                                    F8000640
      IA(3)#IA(1)                                                         F8000650
      W1(1)#ATOMS(2,M)                                                    F8000660
      W1(2)#ATOMS(3,M)                                                    F8000670
      W1(3)#ATOMS(4,M)                                                    F8000680
      L#M+1                                                               F8000690
      DO 895 N#L,LATM                                                     F8000700
      DIST#(ATOMS(2,N)-W1(1))**2                                          F8000710
      IF(DMAX-DIST)895,873,873                                            F8000720
  873 DIST#DIST+(ATOMS(3,N)-W1(2))**2                                     F8000730
      IF(DMAX-DIST)895,874,874                                            F8000740
  874 DIST#DIST+(ATOMS(4,N)-W1(3))**2                                     F8000750
      IF(DMAX-DIST)895,875,875                                            F8000760
  875 DIST#SQRTF(DIST)                                                    F8000770
      T2#ATOMS(1,N)                                                       F8000780
      IA(2)#T2/100000.                                                    F8000790
C     ***** SELECT BONDS ACCORDING TO CODES *****                         F8000800
      DO 890 J#1,NCD                                                      F8000810
      JB#J                                                                F8000820
      IF(DIST-CD(1,J))    890,880,880                                     F8000830
  880 IF(CD(2,J)-DIST)    890,881,881                                     F8000840
  881 DO 885 K#1,2                                                        F8000850
      IF(IA(K)-KD(1,J))   885,882,882                                     F8000860
  882 IF(KD(2,J)-IA(K))   885,883,883                                     F8000870
  883 IF(IA(K+1)-KD(3,J))885,884,884                                      F8000880
  884 IF(KD(4,J)-IA(K+1))885,891,891                                      F8000890
  885 CONTINUE                                                            F8000900
  890 CONTINUE                                                            F8000910
      GO TO 895                                                           F8000920
  891 IF(NJ2-10)892,894,894                                               F8000930
  892 LNS#XMODF(LNS+4,56)                                                 F8000940
      IF(LNS)893,893,894                                                  F8000950
  893 WRITE OUTPUT TAPE NOUT,835,(TITLE(I),I#1,12)                        F8000960
      WRITE OUTPUT TAPE NOUT,837                                          F8000970
  894 CALL BOND(T1,T2,JB)                                                 F8000980
  895 CONTINUE                                                            F8000990
  899 RETURN                                                              F8001000
      END                                                                 F8001010
*LIST8
*LABEL
      SUBROUTINE F900                                                     F9000010
      DIMENSION X(3),XW(3,5),Y(3),Z(3)                                    F9000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      F9000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F9000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F9000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F9000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F9000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F9000080
      DIMENSION XLNG(3),XO(3),XT(3)                                       F9000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F9000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F9000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF9000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F9000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                  F9000140
C     ***** LABELING FUNCTION SUBROUTINE *****                            F9000150
      ITILT#0                                                             F9000160
      NJ3#XMODF(NJ2,10)                                                   F9000170
      TH#THETA                                                            F9000180
      SINTH#SYMB(2,1)                                                     F9000190
      COSTH#SYMB(1,1)                                                     F9000200
      ILAST#1                                                             F9000210
      IF(AIN(2)-11100.)910,910,905                                        F9000220
  905 ILAST#2                                                             F9000230
  910 DO 925 II#1,ILAST                                                   F9000240
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C     ***** OBTAIN WORKING CARTESIAN COORDINATES *****                F9000250
      CALL XYZ(AIN(II),XW(1,II),2)                                     F9000260
      IF(NG)915,925,915                                                F9000270
  912 NG#15                                                            F9000280
  915 CALL ERPNT(AIN(II),NJ*100+NJ2)                                   F9000290
      GO TO 1199                                                       F9000300
  925 CALL XYZ(AIN(II),XW(1,II+3),3)                                   F9000310
      II#1                                                             F9000320
C     ***** FIND MEAN REFERENCE POINT *****                            F9000330
      DO 930 J#1,3                                                     F9000340
      T2#XW(J,ILAST)                                                   F9000350
      T1#XW(J,1)                                                       F9000360
      XW(J,3)#T2-T1                                                    F9000370
  930 X(J)#(T2+T1)*.5                                                  F9000380
C     ***** PERSPECTIVE SCALING FACTOR *****                           F9000390
      SCAL#1.                                                          F9000400
      IF(VIEW)940,940,935                                              F9000410
  935 SCAL#VIEW/(VIEW-X(3))                                            F9000420
  940 HGT#SCAL*AIN(5)                                                  F9000430
      IF(NJ2-3)960,950,945                                             F9000440
  945 IF(NJ2-6)950,950,960                                             F9000450
C     ***** PROJECTED VECTOR BASELINE *****                            F9000460
  950 CALL PLTXY(XW(1,4),V1)                                           F9000470
      CALL PLTXY(XW(1,5),V2)                                           F9000480
      T1#V2(1)-V1(1)                                                   F9000490
      T2#V2(2)-V1(2)                                                   F9000500
      T3#SQRTF(T1*T1+T2*T2)                                            F9000510
      IF(T3)912,912,955                                                F9000520
  955 COSTH#T1/T3                                                      F9000530
      SINTH#T2/T3                                                      F9000540
      TH#ARCCOS(COSTH)                                                 F9000550
      IF(SINTH)958,960,960                                             F9000560
  958 TH#-TH                                                           F9000570
  960 IF(NJ2-13)965,985,985                                            F9000580
C     ***** FIND CENTER OF PROJECTED LABEL *****                       F9000590
  965 Y(1)#SCAL*(X(1)+AIN(6)*COSTH-AIN(7)*SINTH)+XO(1)                 F9000600
      Y(2)#SCAL*(X(2)+AIN(6)*SINTH+AIN(7)*COSTH)+XO(2)                 F9000610
      Y(3)#0.                                                          F9000620
C     ***** CHECK FOR LEGEND RESET *****                               F9000630
      DO 980 J#1,2                                                     F9000640
      T1#AIN(J+2)                                                      F9000650
      IF(T1)975,980,970                                                F9000660
  970 Y(J)#T1                                                          F9000670
      GO TO 980                                                        F9000680
  975 Y(J)#XLNG(J)+T1                                                  F9000690
  980 CONTINUE                                                         F9000700
C     ***** SET PARAMETERS FOR INDIVIDUAL FUNCTIONS *****              F9000710
  985 GO TO(990,995,995,1000,1000,1000,915,1105,1105,915,915,915,1005,1F9000720
     105,1005,1005,915),NJ2                                            F9000730
  990 T6#17.                                                           F9000740
      L#AIN(1)/100000.                                                 F9000750
      ILAST#1                                                          F9000760
      DXW#0.                                                           F9000770
      DYW#0.                                                           F9000780
      GO TO 1030                                                       F9000790
  995 T6#215.                                                          F9000800
      ILAST#12                                                         F9000810
      T1#HGT*36./7.                                                    F9000820
      DXW#COSTH*T1                                                     F9000830
      DYW#SINTH*T1                                                     F9000840
      GO TO 1030                                                       F9000850
 1000 T6#22+3*(6-NJ3)                                                  F9000860
      DIST#SQRTF(VV(XW(1,3),XW(1,3)))/SCAL1                            F9000870
      GO TO 1030                                                       F9000880
C     ***** TRUE PERSPECTIVE LABELS *****                              F9000890
 1005 CALL UNIT(XW(1,3),VT(1,1),1)                                     F9000900
      IF(ABSF(VT(3,1))-.9994)1010,912,912                              F9000910
C     ***** FORM PERSPECTIVE ROTATION MATRIX *****                     F9000920
 1010 CALL NORM(AID(1,3),VT(1,1),VT(1,2),1)                            F9000930
      CALL UNIT(VT(1,2),VT(1,2),1)                                     F9000940
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      CALL NORM(VT(1,1),VT(1,2),VT(1,3),1)                              F9000950
      DO 1015 J#1,3                                                     F9000960
 1015 VT(J,4)#X(J)                                                      F9000970
      ITILT#1                                                           F9000980
      HGT#AIN(5)                                                        F9000990
      TH#0.                                                             F9001000
      Y(3)#X(3)                                                         F9001010
      Y(2)#X(2)+AIN(7)-HGT*.5                                           F9001020
      IF(NJ2-13)1030,1025,1020                                          F9001030
C     ***** PERSPECTIVE BCND LABELS *****                               F9001040
 1020 Y(1)#X(1)+AIN(6)-HGT*FLOATF(22+3*(6-NJ3))/7.                      F9001050
      DIST#SQRTF(VV(XW(1,3),XW(1,3)))/SCALI                             F9001060
      GO TO 1050                                                        F9001070
C     ***** PERSPECTIVE TITLES *****                                    F9001080
 1025 Y(1)#X(1)+AIN(6)-HGT*215./7.                                      F9001090
      ILAST#12                                                          F9001100
      DXW#HGT*36./7.                                                    F9001110
      DYW#0.                                                            F9001120
      GO TO 1050                                                        F9001130
 1030 DH#HGT*T6/7.                                                      F9001140
      DV#HGT*.5                                                         F9001150
      Y(1)#Y(1)-DH*COSTH+DV*SINTH                                       F9001160
      Y(2)#Y(2)-DH*SINTH-DV*COSTH                                       F9001170
      Y(3)#0.                                                           F9001180
C     ***** PLOT VARIOUS LABELS *****                                   F9001190
 1050 GO TO(1060,1060,1060,1090,1095,1100,915,1105,1105),NJ3            F9001200
 1060 DO 1085 I#1,ILAST                                                 F9001210
      DO 1075 J#1,3,2                                                   F9001220
      Z(1)#Y(1)+FLOATF(J-2)*DISP*.5                                     F9001230
      DO 1075 K#1,3,2                                                   F9001240
      Z(2)#Y(2)+FLOATF(K-2)*DISP*.5                                     F9001250
      IF(NJ3-2)1065,1068,1068                                           F9001260
C     ***** PLOT CHEMICAL SYMBOL *****                                  F9001270
 1065 CALL SIMBOL(Z(1),Z(2),HGT,CHEM(L),TH,6)                           F9001280
      GO TO 1070                                                        F9001290
C     ***** PLOT TITLES *****                                           F9001300
 1068 CALL SIMBOL(Z(1),Z(2),HGT,TITLE2(I),TH,6)                         F9001310
 1070 IF(DISP)1080,1080,1075                                            F9001320
 1075 CONTINUE                                                          F9001330
 1080 Y(1)#Y(1)+DXW                                                     F9001340
 1085 Y(2)#Y(2)+DYW                                                     F9001350
      GO TO 1199                                                        F9001360
C     ***** PLOT BCND DISTANCE LABELS *****                             F9001370
 1090 CALL NOMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.1)                         F9001380
      GO TO 1199                                                        F9001390
 1095 CALL NOMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.2)                         F9001400
      GO TO 1199                                                        F9001410
 1100 CALL NOMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.3)                         F9001420
      GO TO 1199                                                        F9001430
C     ***** PLOT CENTERED SYMBOLS *****                                 F9001440
 1105 CALL SIMBOL(Y(1),Y(2),HGT,XFIXF(AIN(8)),TH,7-NJ3)                 F9001450
 1199 ITILT#0                                                           F9001460
      RETURN                                                            F9001470
      END                                                               F9001480
*LIST8
*LABEL
      SUBROUTINE FIOOO                                                  FIOC0010
      RETURN                                                            FIOC0020
      END                                                               FIOC0030
*LIST8
*LABEL
      SUBROUTINE MM(X,Y,Z)                                              MM  0010
C     MULTIPLY TWO MATRICES                                             MM  0020
C     Z(3,3)#X(3,3)*Y(3,3)                                              MM  0030
      DIMENSIONX(3,3),Y(3,3),Z(3,3)                                     MM  0040
      DO117I#1,3                                                        MM  0050
      DO117K#1,3                                                        MM  0060
      Z(I,K)#0.0                                                        MM  0070
      DO117J#1,3                                                        MM  0080
  117 Z(I,K)#Z(I,K)+X(I,J)*Y(J,K)                                       MM  0090
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      RETURN                                                            MM  0100
      END                                                               MM  0110
*LIST8
*LABEL
      SUBROUTINE MV(X,Y,Z)                                              MV  0010
C     MATRIX * VECTOR                                                   MV  0020
C     Z(3)#X(3,3)*Y(3)                                                  MV  0030
      DIMENSIONX(3,3),Y(3),Z(3)                                         MV  0040
      DO113I#1,3                                                        MV  0050
      Z(I)#0.0                                                          MV  0060
      DO113J#1,3                                                        MV  0070
  113 Z(I)#Z(I)+X(I,J)*Y(J)                                             MV  0080
      RETURN                                                            MV  0090
      END                                                               MV  0100
*LIST8
*LABEL
      SUBROUTINE NORM(X,Y,Z,ITYPE)                                      NORM0010
C     ***** VECTOR PRODUCT  Z#X*Y *****                                 NORM0020
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         NORM0030
      DIMENSION X(3),Y(3),Z(3,3),ZI(3,3)                                NORM0040
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    NORM0050
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)NORM0060
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) NORM0070
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) NORM0080
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   NORM0090
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   NORM0100
      DIMENSION XLNG(3),XO(3),XT(3)                                     NORM0110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   NORM0120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD NORM0130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALINORM0140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   NORM0150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                NORM0160
      DO 125 I#1,3                                                      NORM0170
      I1#XMODF(I+3,3)+1                                                 NORM0180
      I2#XMODF(I+1,3)+1                                                 NORM0190
      T1#X(I1)*Y(I2)-X(I2)*Y(I1)                                        NORM0200
      IF(ITYPE)115,115,105                                              NORM0210
  105 Z(I)#T1                                                           NORM0220
      GO TO 125                                                         NORM0230
  115 Z1(I)#T1                                                          NORM0240
  125 CONTINUE                                                          NORM0250
      IF(ITYPE)135,135,300                                              NORM0260
  135 CALL MV(BB,Z1,Z)                                                  NORM0270
  300 RETURN                                                            NORM0280
      END                                                               NORM0290
*LIST8
*LABEL
      SUBROUTINE PAXES(ACODE,ITYPE)                                     PAXE0010
C     ***** ITYPE .LT.0 FOR COVARIANCE MATRIX IN Q *****                PAXE0020
C     ***** ITYPE .GT.0 FOR ELLIPSOID QUADRATIC FORM IN Q *****         PAXE0030
C     ***** XABSF(ITYPE)#1 BASED ON TRICLINIC COORDINATE SYSTEM *****   PAXE0040
C     ***** #2 OR 3 FOR WORKING OR REFERENCE CARTESIAN SYSTEMS *****    PAXE0050
C     ***** CHECK ATOM CODE *****                                       PAXE0060
      DIMENSION W(3,3),X(3)                                             PAXE0070
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PAXE0080
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PAXE0090
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PAXE0100
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PAXE0110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PAXE0120
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PAXE0130
      DIMENSION XLNG(3),XO(3),XT(3)                                     PAXE0140
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PAXE0150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PAXE0160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPAXE0170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PAXE0180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PAXE0190
      IT#XABSF(ITYPE)-1                                                 PAXE0200
      KS#MODF(ACODE,100.)                                               PAXE0210
      IF(NSYM-KS)105,115,115                                            PAXE0220
  105 NG#4                                                              PAXE0230
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      GO TO 300                                                         PAXE0240
  115 II#ACODE/100000.                                                  PAXE0250
      IF(NATOM-II)125,130,130                                           PAXE0260
  125 NG#5                                                              PAXE0270
      GO TO 300                                                         PAXE0280
  130 IF(II)125,125,135                                                 PAXE0290
C     ***** CRYSTALLOGRAPHIC SYMMETRY ROTATION *****                    PAXE0300
  135 CALL TMM(PA(1,1,II),FS(1,1,KS),PAT)                               PAXE0310
      IF(IT-1)165,145,155                                               PAXE0320
C     ***** TRANSFORM TO CARTESIAN SYSTEMS *****                        PAXE0330
  145 CALL TMM(PAT,AAWRK,PAC)                                           PAXE0340
      GO TO 175                                                         PAXE0350
  155 CALL TMM(PAT,AAREV,PAC)                                           PAXE0360
      GO TO 175                                                         PAXE0370
  165 IF(ITYPE)170,175,170                                              PAXE0380
C     ***** (PAT)**(-1) * (AA)**(-1) *****                              PAXE0390
  170 CALL AXEQB(PAT,W,BB,3)                                            PAXE0400
C     ***** FORM DIAGONAL MATRIX OR ITS INVERSE *****                   PAXE0410
  175 DO 205 J#1,3                                                      PAXE0420
      TI#EV(J,II)                                                       PAXE0430
      IF(ITYPE)195,205,185                                              PAXE0440
  185 X(J)#1./(TI*TI)                                                   PAXE0450
      GO TO 205                                                         PAXE0460
  195 X(J)#TI*TI                                                        PAXE0470
  205 RMS(J)#TI                                                         PAXE0480
C     ***** FORM QUADRATIC FORM *****                                   PAXE0490
      DO 245 I#1,3                                                      PAXE0500
      DO 245 J#1,3                                                      PAXE0510
      TI#0.0                                                            PAXE0520
      IF(IT)300,210,220                                                 PAXE0530
  210 DO 215 K#1,3                                                      PAXE0540
C     ***** BASED ON TRICLINIC SYSTEM *****                             PAXE0550
  215 TI#TI+PAT(I,K)*W(K,J)*X(K)                                        PAXE0560
      GO TO 235                                                         PAXE0570
C     ***** BASED ON CARTESIAN SYSTEM *****                             PAXE0580
  220 DO 225 K#1,3                                                      PAXE0590
  225 TI#TI+PAC(I,K)*PAC(J,K)*X(K)                                      PAXE0600
  235 Q(J,I)#TI                                                         PAXE0610
  245 Q(I,J)#TI                                                         PAXE0620
  300 RETURN                                                            PAXE0630
      END                                                               PAXE0640
*LIST8
*LABEL
      SUBROUTINE PLTXY(X,Y)                                             PLTX0010
C     ***** PLOT COORD. AND CLOSEST EDGE AFTER PROJECTION *****         PLTX0020
      DIMENSION X(3),Y(2)                                               PLTX0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PLTX0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PLTX0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PLTX0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PLTX0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PLTX0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PLTX0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     PLTX0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PLTX0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PLTX0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPLTX0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PLTX0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PLTX0150
      T4#1.                                                             PLTX0160
      TI#1.                                                             PLTX0170
      IF(VIEW)125,125,110                                               PLTX0180
  110 T4#VIEW-X(3)                                                      PLTX0190
      IF(T4)115,115,120                                                 PLTX0200
  115 Y(1)#-99.                                                         PLTX0210
      Y(2)#-99.                                                         PLTX0220
      GO TO 130                                                         PLTX0230
  120 TI#VIEW/T4                                                        PLTX0240
  125 Y(1)#X(1)*TI+XO(1)                                                PLTX0250
      Y(2)#X(2)*TI+XO(2)                                                PLTX0260
      TI#XLNG(1)-ABSF(Y(1)*2.-XLNG(1))                                  PLTX0270
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      T2#XLNG(2)-ABSF(Y(2)*2.-XLNG(2))                                  PLTX0280
      EDGE#MINIF(T1,T2)*.5                                              PLTX0290
      IF(T4-VIEW*.5)130,300,300                                         PLTX0300
  130 EDGE#-99.                                                         PLTX0310
  300 RETURN                                                            PLTX0320
      END                                                               PLTX0330
*LIST8
*LABEL
      SUBROUTINE PRELIM                                                 PREL0010
C     ***** DATA INPUT ROUTINE *****                                    PREL0020
      DIMENSION B(9)                                                    PREL0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PREL0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PREL0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PREL0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PREL0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PREL0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PREL0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     PREL0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PREL0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATN,LTNO,NATOM,NCD PREL0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPREL0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PREL0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PREL0150
C     ***** CELL DIMENSIONS *****                                       PREL0160
  106 FORMAT(6F9.6)                                                     PREL0170
      READ INPUT TAPE IN,106,(A(I),I#1,6)                               PREL0180
      T1#ABSF(A(4))-1.                                                  PREL0190
      DO 125 J#1,3                                                      PREL0200
      IF(T1)115,110,110                                                 PREL0210
C     ***** CELL ANGLES IN DEGREES *****                                PREL0220
  110 A(J+6)#A(J+3)                                                     PREL0230
      A(J+3)#COSF(A(J+6)*.01745329252)                                  PREL0240
      GO TO 120                                                         PREL0250
C     ***** COSINES OF CELL ANGLES *****                                PREL0260
  115 A(J+6)#ARCCOS(A(J+3))                                             PREL0270
C     ***** STORE IDEMFACTOR MATRIX *****                               PREL0280
  120 AID(J,J)#1.                                                       PREL0290
      AID(J+1,1)#0.                                                     PREL0300
      AID(J+5,1)#0.                                                     PREL0310
C     ***** STORE METRIC TENSOR *****                                   PREL0320
  125 AA(J,J)#A(J)**2                                                   PREL0330
      AA(1,2)#A(1)*A(2)*A(6)                                            PREL0340
      AA(1,3)#A(1)*A(3)*A(5)                                            PREL0350
      AA(2,3)#A(2)*A(3)*A(4)                                            PREL0360
      AA(2,1)#AA(1,2)                                                   PREL0370
      AA(3,1)#AA(1,3)                                                   PREL0380
      AA(3,2)#AA(2,3)                                                   PREL0390
C     ***** INVERT METRIC TENSOR *****                                  PREL0400
      CALL AXEQB(AA,BB,AID,3)                                           PREL0410
C     ***** CALCULATE RECIPROCAL CELL PARAMETERS *****                  PREL0420
      DO 128 J#1,3                                                      PREL0430
  128 B(J)#SQRTF(BB(J,J))                                               PREL0440
      B(6)#BB(1,2)/(B(1)*B(2))                                          PREL0450
      B(5)#BB(1,3)/(B(1)*B(3))                                          PREL0460
      B(4)#BB(2,3)/(B(2)*B(3))                                          PREL0470
      DO 130 J#1,3                                                      PREL0480
  130 B(J+6)#ARCCOS(B(J+3))                                             PREL0490
C     ***** WAS INPUT FOR REAL OR RECIPROCAL CELL *****                 PREL0500
      IF(A(1)-1.)135,150,150                                            PREL0510
  135 DO 140 J#1,9                                                      PREL0520
      T1#AA(J,1)                                                        PREL0530
      AA(J,1)#BB(J,1)                                                   PREL0540
      BB(J,1)#T1                                                        PREL0550
      T1#A(J)                                                           PREL0560
      A(J)#B(J)                                                         PREL0570
  140 B(J)#T1                                                           PREL0580
C     ***** WRITE OUT CELL PARAMETERS *****                             PREL0590
  143 FORMAT(1H0 10X,22HDIRECT CELL PARAMETERS/1H 15X,1HA14X,1HB14X,1HC14PREL0600
     1X,5HALPHA10X,4HBETA11X,5HGAMMA)                                   PREL0610
  145 FORMAT(1H 10X,F9.6,2F15.6,3F15.3/1H 48X,6HCOSINEF12.8,2F15.8)     PREL0620
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  147 FORMAT(1H010X,26HRECIPROCAL CELL PARAMETERS/1H 15X,2HA*13X,2HB*13XPREL0630
     1,2HC*13X,6HALPHA*9X,5HBETA*10X,6HGAMMA*)                          PREL0640
  150 WRITE OUTPUT TAPE NOUT,143                                        PREL0650
      WRITE OUTPUT TAPE NOUT,145,(A(I),I#1,3),(A(I),I#7,9),(A(I),I#4,6) PREL0660
      WRITE OUTPUT TAPE NOUT,147                                        PREL0670
      WRITE OUTPUT TAPE NOUT,145,(B(I),I#1,3),(B(I),I#7,9),(B(I),I#4,6) PREL0680
C     ***** STORE STANDARD VECTORS *****                                PREL0690
      CALL AXES(AID,AID(1,2),REFV,0)                                    PREL0700
      CALL MM(AA,REFV,AAREV)                                            PREL0710
      DO 160 I#1,3                                                      PREL0720
      DO 160 J#1,3                                                      PREL0730
      AAWRK(J,I)#AAREV(J,I)                                             PREL0740
      Q(J,I)#REFV(I,J)                                                  PREL0750
  160 WRKV(J,I)#REFV(J,I)                                               PREL0760
C     ***** READ AND WRITE SYMMETRY TRANSFORMATIONS *****               PREL0770
  171 FORMAT(1H010X,24HSYMMETRY TRANSFORMATIONS/1H 14X,3HNO.12X,13HTRANSPREL0780
     1FORMED X18X,13HTRANSFORMED Y18X,13HTRANSFORMED Z)                 PREL0790
  173 FORMAT(I1,F14.10,3F3.0,2(F15.10,3F3.0))                           PREL0800
  175 FORMAT(1H 13X,I2,3(F13.6,F4.0,2H XF4.0,2H YF4.0,2H Z))            PREL0810
  177 FORMAT(1H110X,12A6)                                               PREL0820
      WRITE OUTPUT TAPE NOUT,171                                        PREL0830
      LINES#14                                                          PREL0840
      DO 190 I#1,48                                                     PREL0850
      LINES#XMODF(LINES+1,56)                                           PREL0860
      READ INPUT TAPE IN,173,IS,(TS(J,I),(FS(K,J,I),K#1,3),J#1,3)       PREL0870
      IF(LINES)185,180,185                                              PREL0880
  180 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12)                      PREL0890
      WRITE OUTPUT TAPE NOUT,171                                        PREL0900
  185 WRITE OUTPUT TAPE NOUT,175,I,(TS(J,I),(FS(K,J,I),K#1,3),J#1,3)    PREL0910
C     ***** NON-CRYSTALLOGRAPHIC HELIX-SYMMETRY INPUT *****             PREL0920
      IF(FS(3,3,I)-5.)188,186,186                                       PREL0930
  186 T1#FS(1,3,I)/FS(3,3,I)                                            PREL0940
      TS(3,I)#TS(3,I)+T1                                                PREL0950
      T1#MODF(T1*FS(2,3,I),1.)*6.28318531                               PREL0960
      T2#COSF(T1)                                                       PREL0970
      T1#SINF(T1)                                                       PREL0980
      DO 187 J#1,9                                                      PREL0990
  187 VT(J,I)#AID(J,I)                                                  PREL1000
      VT(1,1)#T2                                                        PREL1010
      VT(2,2)#T2                                                        PREL1020
      VT(2,1)#-T1                                                       PREL1030
      VT(1,2)#T1                                                        PREL1040
      CALL MM(VT,Q,PAC)                                                 PREL1050
      CALL MM(AAREV,PAC,FS(1,1,I))                                      PREL1060
  188 IF(IS)195,190,195                                                 PREL1070
  190 CONTINUE                                                          PREL1080
      NG#1                                                              PREL1090
      CALL ERPNT(0.,0)                                                  PREL1100
      I#48                                                              PREL1110
  195 NSYM#I                                                            PREL1120
C     ***** POSITIONAL AND THERMAL PARAMETERS *****                     PREL1130
  207 FORMAT(11H0 NO. ATOM 8X,1HX10X,1HY10X,1HZ13X,3HB118X,3HB228X,3HB33PREL1140
     18X,3HB128X,3HB138X,10HB23   TYPE)                                 PREL1150
  209 FORMAT(1H I3,1X,A6,3F11.6,5X,6F11.6,F5.0)                         PREL1160
  210 FORMAT(1H I3,1X,A6,3F11.6,5X,2F11.6,4F11.0,F5.0)                  PREL1170
  211 FORMAT(A6,3X,5F9.6,F9.0)                                          PREL1180
  213 FORMAT(I1,F8.6,5F9.6,F9.0)                                        PREL1190
      LINES#LINES+2                                                     PREL1200
      IF(LINES-56)220,215,215                                           PREL1210
  215 LINES#-1                                                          PREL1220
      GO TO 225                                                         PREL1230
  220 WRITE OUTPUT TAPE NOUT,207                                        PREL1240
  225 DO 245 I#1,200                                                    PREL1250
      LINES#XMODF(LINES+1,56)                                           PREL1260
      READ INPUT TAPE IN,211,CHEM(I),V1(1),V1(2),(P(J,I),J#1,3),T1      PREL1270
      K#1.+T1                                                           PREL1280
      READ INPUT TAPE IN,213,IS,(PA(J,1,I),J#1,7)                       PREL1290
      IF(LINES)230,230,232                                              PREL1300
  230 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12)                      PREL1310
      WRITE OUTPUT TAPE NOUT,207                                        PREL1320
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```
  232 IF(PA(3,1,I)-10000.)235,234,234                                   PREL1330
  234 WRITE OUTPUT TAPE NOUT,210,I,CHEM(I),(P(J,I),J#1,3),(PA(J,1,I),J#1PREL1340
     1,7)                                                               PREL1350
      GO TO 238                                                         PREL1360
  235 WRITE OUTPUT TAPE NOUT,209,I,CHEM(I),(P(J,I),J#1,3),(PA(J,1,I),J#1PREL1370
     1,7)                                                               PREL1380
  238 GO TO (244,239,241,242,244),K                                     PREL1390
C     ***** TYPE 1 POSITICNAL PARAMETERS (ANGSTROMS) *****              PREL1400
  239 DO 240 J#1,3                                                      PREL1410
  240 P(J,I)#P(J,I)/A(J)                                                PREL1420
      GO TO 244                                                         PREL1430
C     ***** TYPE 2 POSITICNAL PARAMETERS, STANDARD CARTESIAN *****      PREL1440
  241 VI(1)#P(1,I)                                                      PREL1450
      VI(2)#P(2,I)                                                      PREL1460
      GO TO 243                                                         PREL1470
C     ***** TYPE 3 POSITICNAL PARAMETERS *****                          PREL1480
C     ***** CYLINDRICAL COORDINATES REFERRED TO STANDARD CARTESIAN *****PREL1490
  242 T2#P(2,I)*.01745329252                                            PREL1500
      VI(1)#VI(1)+P(1,I)*COSF(T2)                                       PREL1510
      VI(2)#VI(2)+P(1,I)*SINF(T2)                                       PREL1520
  243 VI(3)#P(3,I)                                                      PREL1530
      CALL VM(VI,Q,P(1,I))                                              PREL1540
  244 IF(IS)246,245,246                                                 PREL1550
  245 CONTINUE                                                          PREL1560
      NG#2                                                              PREL1570
      CALL ERPNT(0.,0)                                                  PREL1580
      I#200                                                             PREL1590
  246 NATOM#I                                                           PREL1600
C     ***** CONVERT TEMP FACTOR COEF TO STANDARD TYPE ZERO *****        PREL1610
      NGI#0                                                             PREL1620
      DO 450 I#1,NATOM                                                  PREL1630
      TI#PA(1,1,I)                                                      PREL1640
      K#1.+PA(7,1,I)                                                    PREL1650
      IF(TI)250,250,255                                                 PREL1660
  250 TI#.1                                                             PREL1670
      GO TO 405                                                         PREL1680
  255 T6#.0506605918                                                    PREL1690
      GO TO(270,260,265,265,270,260,400,405,999),K                      PREL1700
C     ***** TYPE 1 *****                                                PREL1710
  260 DO 262 J#4,6                                                      PREL1720
  262 PA(J,1,I)#PA(J,1,I)*.5                                            PREL1730
      GO TO 270                                                         PREL1740
C     ***** TYPES 2 AND 3 (BASE 2 SYSTEMS) *****                        PREL1750
  265 T6#.351152464                                                     PREL1760
      IF(K-4)270,260,270                                                PREL1770
C     ***** TYPES 0 THROUGH 5 *****                                     PREL1780
  270 IF(PA(2,1,I))400,400,272                                          PREL1790
  272 DO 300 J#1,3                                                      PREL1800
      DO 300 L#J,3                                                      PREL1810
      T2#T6                                                             PREL1820
      IF(K-5)285,275,275                                                PREL1830
C     ***** TYPES 4 AND 5 *****                                         PREL1840
  275 T2#B(J)*B(L)*T2*.25                                               PREL1850
  285 IF(J-L)290,282,290                                                PREL1860
  282 VT(J,J)#T2*PA(J,1,I)                                              PREL1870
      GO TO 300                                                         PREL1880
  290 M#J+L+1                                                           PREL1890
      VT(J,L)#T2*PA(M,1,I)                                              PREL1900
      VT(L,J)#VT(J,L)                                                   PREL1910
  300 CONTINUE                                                          PREL1920
C     ***** FIND PRINCIPAL AXES *****                                   PREL1930
      CALL MM(VT,AA,DA)                                                 PREL1940
      CALL EIGEN(DA,RMS,PAT)                                            PREL1950
C     ***** ARE EIGENVALUES POSITIVE *****                              PREL1960
      IF(RMS(1))325,325,320                                             PREL1970
  320 IF(NG)350,360,330                                                 PREL1980
  325 NG#3                                                              PREL1990
  330 NGI#1                                                             PREL2000
      CALL ERPNT(FLOATF(I)*100000.+55501.,0)                            PREL2010
C     ***** 3 EQUAL EIGENVALUES, USE REFERENCE VECTORS *****            PREL2020
```

```
  340 T3#SIGNF(SQRTF(ABSF(RMS(1)+RMS(2)+RMS(3))/3.),RMS(1))
      DO 345 J#1,3
      DO 342 K#1,3
  342 PA(J,K,I)#REFV(J,K)
  345 EV(J,I)#T3
      GO TO 450
  350 IF(NG+6)340,340,352
C     ***** TWO EQUAL EIGENVALUES *****
  352 N#NG+5
      CALL UNIT(PAT(1,N),V1,-1)
      DO 354 K#1,3
      IF(ABSF(VMV(V1,AA,REFV(1,K)))-.58)356,354,354
  354 CONTINUE
  356 CALL MM(AA,DA,VT)
      CALL AXES(V1,REFV(1,K),DA,-1)
      DO 359 K#1,3
      L#XMODF(N+K-2,3)+1
      DO 358 J#1,3
  358 PA(J,L,I)#DA(J,K)
  359 EV(L,I)#SIGNF(SQRTF(ABSF(VMV(DA(1,K),VT,DA(1,K)))),RMS(L))
      GO TO 450
C     ***** MAKE EIGENVECTORS 1 ANGSTROM LONG *****
  360 DO 365 J#1,3
  365 CALL UNIT(PAT(1,J),PA(1,J,I),-1)
  370 NG#0
C     ***** SQRT EIGENVALUE # RMS DISPLACEMENT *****
      DO 375 J#1,3
      T2#RMS(J)
  375 EV(J,I)#SIGNF(SQRTF(ABSF(T2)),T2)
      GO TO 450
C     ***** TYPE 6 (ISOTROPIC TEMP FACTOR) *****
  400 T1#SQRTF(T1*.012665148)
C     ***** TYPE 7 (DUMMY SPHERE) *****
  405 DO 410 J#1,3
  410 EV(J,I)#T1
      IF(PA(3,1,I))430,430,415
C     ***** DEFINED VECTORS FOR SPHERE *****
  415 DO 425 J#1,4
      T2#PA(J+2,1,I)
      CALL ATOM(T2,VT(1,J))
      IF(NG)420,425,420
  420 CALL ERPNT(T2,0)
      GO TO 430
  425 CCONTINUE
      CALL DIFV(VT(1,2),VT(1,1),V1)
      CALL DIFV(VT(1,4),VT(1,3),V2)
      CALL AXES(V1,V2,PA(1,1,I),-1)
      GO TO 450
C     ***** REFERENCE VECTORS FOR SPHERE *****
  430 DO 435 J#1,9
  435 PA(J,1,I)#REFV(J,1)
  450 NG#0
C     ***** WRITE OUT RMS VALUES *****
      LINES#LINES+2
      IF(LINES-56)458,458,455
  455 LINES#-1
      GO TO 460
  458 WRITE OUTPUT TAPE NOUT,461
  460 DO 465 I#1,NATOM
      LINES#XMODF(LINES+1,56)
      IF(LINES)465,462,465
  461 FORMAT(10HONO. ATOM 8X,1HX10X,1HY10X,1HZ13X,7HRMSD 1 4X,7HRMSD 2 4
     1X,7HRMSD 3 )
  462 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12)
      WRITE OUTPUT TAPE NOUT,461
  463 FORMAT(1H I3,1X,A6,3F11.6)
  465 WRITE OUTPUT TAPE NOUT,209,I,CHEM(I),(P(J,I),J#1,3),(EV(J,I),J#1,3
     1)
      IF(NG1)999,999,470
  470 CALL EXIT
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  999 RETURN                                                            PREL2730
      END                                                               PREL2740
*LIST8
*LABEL
      SUBROUTINE PRIME                                                  PRIM0010
C     ****GENERAL INITIALIZATICN OF PRIME PARAMETERS****                PRIM0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PRIM0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PRIM0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PRIM0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PRIM0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PRIM0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PRIM0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     PRIM0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PRIM0100
      COMMCN DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PRIM0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPRIM0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PRIM0130
      COMMCN V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PRIM0140
      BRDR#0.5                                                          PRIM0150
C     ****CALCULATE CONSTANTS****                                       PRIM0160
      DO 2999 I#1,5                                                     PRIM0170
 2999 CONT(I)#SQRTF(1./(2.*(1.+COSF(3.141592654/2.**I))))               PRIM0180
      DISP#.005                                                         PRIM0190
      FORE#.866                                                         PRIM0200
      IN#10                                                             PRIM0210
      ITILT#0                                                           PRIM0220
      LATM#0                                                            PRIM0230
      LTNO#23                                                           PRIM0240
      NCD#0                                                             PRIM0250
      NG#0                                                              PRIM0260
      NOUT#9                                                            PRIM0270
      NSR#11                                                            PRIM0280
      RES(1)#1.25                                                       PRIM0290
      RES(2)#.5                                                         PRIM0300
      RES(3)#.2                                                         PRIM0310
      SCAL1#1.0                                                         PRIM0320
      SCAL2#1.54                                                        PRIM0330
      SCL#1.54                                                          PRIM0340
      DO 3000 I#1,3                                                     PRIM0350
      SYMB(I,I)#1.                                                      PRIM0360
      SYMB(I+1,I)#0.                                                    PRIM0370
 3000 SYMB(I+5,I)#0.                                                    PRIM0380
      TAPER#.375                                                        PRIM0390
      THETA#0.0                                                         PRIM0400
      VIEW#0.0                                                          PRIM0410
      XLNG(1)#30.0                                                      PRIM0420
      XLNG(2)#11.0                                                      PRIM0430
      XO(1)#15.0                                                        PRIM0440
      XO(2)#5.5                                                         PRIM0450
      RETURN                                                            PRIM0460
      END                                                               PRIM0470
*LIST8
*LABEL
      SUBROUTINE PROJ(D,DP,X,XO,VIEW,I1,I2,I3)                          PROJ0010
C     ***** 3D CARTESIAN TO 2D PLOTTER COORDINATES *****                PROJ0020
      DIMENSION D(3,129),DP(2,129),X(3),XO(3)                           PROJ0030
      T3#VIEW-X(3)                                                      PROJ0040
      DO 145 I#I1,I2,I3                                                 PROJ0050
      T1#D(1,I)+X(1)                                                    PROJ0060
      T2#D(2,I)+X(2)                                                    PROJ0070
      IF(VIEW)135,135,120                                               PROJ0080
  120 T4#VIEW/(T3-D(3,I))                                               PROJ0090
      T1#T1*T4                                                          PROJ0100
      T2#T2*T4                                                          PROJ0110
  135 DP(1,I)#T1+XO(1)                                                  PROJ0120
  145 DP(2,I)#T2+XO(2)                                                  PROJ0130
      RETURN                                                            PROJ0140
      END                                                               PROJ0150
*LIST8
*LABEL
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      SUBROUTINE RADIAL(ND)                                             RADI0010
C     ***** GENERATE ELLIPSE FROM TWO CONJUGATE VECTORS *****           RADI0020
C     ***** ORTHONORMAL VECTORS PRODUCE 8-128 SPOKED CIRCLE *****       RADI0030
C     ***** ND DENOTES NUMBER OF SUBDIVISIONS (1 TO 5) *****            RADI0040
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    RADI0050
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)RADI0060
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) RADI0070
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) RADI0080
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   RADI0090
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   RADI0100
      DIMENSION XLNG(3),XO(3),XT(3)                                     RADI0110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   RADI0120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD RADI0130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIRADI0140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   RADI0150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                RADI0160
      DO 115 J#1,3                                                      RADI0170
      T1#DA(J,1)                                                        RADI0180
      D(J,1)#T1                                                         RADI0190
      D(J,129)#T1                                                       RADI0200
      D(J,65)#-T1                                                       RADI0210
      T1#DA(J,2)                                                        RADI0220
      D(J,33)#T1                                                        RADI0230
  115 D(J,97)#-T1                                                       RADI0240
      DO 135 K#1,ND                                                     RADI0250
      T1#CONT(K)                                                        RADI0260
      KDEL#2**(6-K)                                                     RADI0270
      KDEL1#KDEL+1                                                      RADI0280
      KDEL2#KDEL/2                                                      RADI0290
      DO 135 L#KDEL1,65,KDEL                                            RADI0300
      J#L-KDEL                                                          RADI0310
      M#L-KDEL2                                                         RADI0320
      DO 135 N#1,3                                                      RADI0330
      T2#(D(N,L)+D(N,J))*T1                                             RADI0340
      D(N,M)#T2                                                         RADI0350
  135 D(N,M+64)#-T2                                                     RADI0360
      RETURN                                                            RADI0370
      END                                                               RADI0380
*LIST8
*LABEL
      SUBROUTINE SEARCH                                                 SEAR0010
      DIMENSION NW(6),DX(3),S(2,200),U(3),V(3),W(2,4),WW(2,3),X(4),Y(3) SEAR0020
      DIMENSION Z(3)                                                    SEAR0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    SEAR0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)SEAR0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) SEAR0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) SEAR0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   SEAR0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   SEAR0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     SEAR0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   SEAR0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD SEAR0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALISEAR0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   SEAR0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                SEAR0150
      EQUIVALENCE(NW(1),LL),(NW(2),LU),(NW(3),ML)                       SEAR0160
      EQUIVALENCE(NW(4),MU),(NW(5),NL),(NW(6),NU)                       SEAR0170
C     ***** OBTAIN PROBLEM PARAMETERS *****                             SEAR0180
      WRITE OUTPUT TAPE NOUT,20                                         SEAR0190
   20 FORMAT(1H0 9X,82H       FROM ATOMS     TO ATOMS        WITH RADIUS ORSEAR0200
     1, IF A BOX, WITH SEMIDIMENSIONS  /11X,46HCODE (MIN   MAX)    (MIN   MSEAR0210
     2AX)                    7X,1HA8X,1HB8X,1HC)                        SEAR0220
      IF(AIN(1)-10000.)100,100,101                                      SEAR0230
  100 ITCM1#AIN(1)                                                      SEAR0240
      SYITOM#55501.                                                     SEAR0250
      GO TO 103                                                         SEAR0260
  101 ITCM1#AIN(1)/100000.                                              SEAR0270
      SYITOM#MODF(AIN(1),100000.)                                       SEAR0280
  102 IF(AIN(2)-10000.)103,103,104                                      SEAR0290
  103 ITCM2#AIN(2)                                                      SEAR0300
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      GO TO 105                                                         SEAR0310
  104 ITOM2#AIN(2)/100000.                                              SEAR0320
  105 ITAR1#AIN(3)                                                      SEAR0330
      IF(ITAR1)108,108,110                                              SEAR0340
  108 ITAR1#1                                                           SEAR0350
  110 ITAR2#AIN(4)                                                      SEAR0360
      DMAX#AIN(5)                                                       SEAR0370
      IF(DMAX)115,115,120                                               SEAR0380
  115 DMAX#4.                                                           SEAR0390
      AIN(5)#DMAX                                                       SEAR0400
  120 DMX#DMAX*DMAX                                                     SEAR0410
      TEM#.01                                                           SEAR0420
      KFUN#NJ*100+XMODF(NJ2,10)                                         SEAR0430
      K#NJ*100+NJ2                                                      SEAR0440
      I0#SYITOM                                                         SEAR0450
  121 FORMAT(1H010X,2I3,2I5,I7,I5,18X,3F9.3/1H )                        SEAR0460
      WRITE OUTPUT TAPE NOUT,121,K,ITOM1,I0,ITOM2,ITAR1,ITAR2,(AIN(J),J#SEAR0470
     15,7)                                                              SEAR0480
  124 FORMAT(1H 15X,2I5,I8,I5,2F9.3)                                    SEAR0490
      IF(NCD)130,130,125                                                SEAR0500
  125 WRITE OUTPUT TAPE NOUT,124,(((KD(J,I),J#1,4),(CD(J,I),J#1,2)),I#1,SEAR0510
     1NCD)                                                              SEAR0520
  130 DO 135 J#1,4                                                      SEAR0530
      W(1,J)#99.                                                        SEAR0540
  135 W(2,J)#-99.                                                       SEAR0550
      DO 155 I#ITAR1,ITAR2                                              SEAR0560
      T1#FLOATF(I)*100000.                                              SEAR0570
      CALL ATOM(T1,X)                                                   SEAR0580
      IF(NG)140,145,140                                                 SEAR0590
  140 CALL ERPNT(T1,KFUN)                                               SEAR0600
      GO TO 600                                                         SEAR0610
  145 X(4)#X(1)-X(2)                                                    SEAR0620
      DO 155 J#1,4                                                      SEAR0630
      TEM#X(J)                                                          SEAR0640
      IF(W(2,J)-TEM)148,150,150                                         SEAR0650
  148 W(2,J)#TEM                                                        SEAR0660
  150 IF(TEM-W(1,J))152,155,155                                         SEAR0670
  152 W(1,J)#TEM                                                        SEAR0680
  155 CONTINUE                                                          SEAR0690
      IF(KFUN-403)165,160,600                                           SEAR0700
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES MODEL BOX *****          SEAR0710
  160 DO 162 J#1,3                                                      SEAR0720
      DX(J)#0.                                                          SEAR0730
      DO 162 I#1,3                                                      SEAR0740
  162 DX(J)#DX(J)+ABSF(REFV(J,I)*AIN(I+4))                              SEAR0750
      GO TO 170                                                         SEAR0760
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES DMAX SPHERE *****        SEAR0770
  165 T1#1.-A(4)*A(4)-A(5)*A(5)-A(6)*A(6)+2.*A(4)*A(5)*A(6)             SEAR0780
      DO 168 J#1,3                                                      SEAR0790
  168 DX(J)#SQRTF((1.-A(J+3)**2)/T1)*DMAX/A(J)                          SEAR0800
C     ***** START SEARCH AROUND REFERENCE ATOMS *****                   SEAR0810
  170 DO 500 ITOM#ITOM1,ITOM2                                           SEAR0820
      T1#FLOATF(ITOM)*100000.+SYITOM                                    SEAR0830
      CALL ATOM(T1,Y)                                                   SEAR0840
      IF(NG)171,172,171                                                 SEAR0850
  171 CALL ERPNT(T1,KFUN)                                               SEAR0860
      GO TO 500                                                         SEAR0870
C     ***** K#SYMMETRY EQUIVALENT POSITION *****                        SEAR0880
  172 NUM#0                                                             SEAR0890
  173 DO 400 K#1,NSYM                                                   SEAR0900
C     ***** SUBTRACT SYMMETRY TRANSLATION FROM REF ATOM *****           SEAR0910
      DO 175 J#1,3                                                      SEAR0920
  175 U(J)#Y(J)-TS(J,K)                                                 SEAR0930
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****               SEAR0940
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****     SEAR0950
      DO 185 J#1,3                                                      SEAR0960
      DO 185 L#1,2                                                      SEAR0970
      WW(L,J)#0.0                                                       SEAR0980
      DO 185 I#1,3                                                      SEAR0990
      TEM#FS(I,J,K)                                                     SEAR1000
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      IF(TEM)177,185,179                                                SEAR1010
  177 N#XMODF(L,2)+1                                                    SEAR1020
      GO TO 183                                                         SEAR1030
  179 N#L                                                               SEAR1040
  183 WW(L,J)#WW(L,J)+W(N,I)*TEM                                        SEAR1050
  185 CONTINUE                                                          SEAR1060
C     ***** CHECK FOR MIXED INDEX TRANSFORMATION *****                  SEAR1070
      DO 215 J#1,2                                                      SEAR1080
      TEM#FS(1,J,K)                                                     SEAR1090
      IF(TEM+FS(2,J,K))215,201,215                                      SEAR1100
  201 IF(TEM)203,215,207                                                SEAR1110
  203 WW(1,J)#W(2,4)*TEM                                                SEAR1120
      WW(2,J)#W(1,4)*TEM                                                SEAR1130
      GO TO 215                                                         SEAR1140
  207 WW(1,J)#W(1,4)*TEM                                                SEAR1150
      WW(2,J)#W(2,4)*TEM                                                SEAR1160
  215 CONTINUE                                                          SEAR1170
C     ***** MOVE 4 CELLS AWAY THEN MOVE BACK UNTIL PARALLELEPIPED AROUNDSEAR1180
C         REF ATOM AND BOX AROUND TRANSFORMED ASYM UNIT INTERSECT ***** SEAR1190
      N#0                                                               SEAR1200
      DO 235 J#1,3                                                      SEAR1210
      DO 225 I#1,2                                                      SEAR1220
      N#N+1                                                             SEAR1230
      TT#(U(J)-WW(I,J))*FLOATF(I*2-3)-DX(J)                             SEAR1240
      TEM#5.0                                                           SEAR1250
  221 TEM#TEM-1.0                                                       SEAR1260
      IF(TEM+TT)225,225,221                                             SEAR1270
  225 NW(N)#TEM*FLOATF(I*2-3)+5.                                        SEAR1280
C     ***** IF NO POSSIBILITY OF A HIT, GO TO NEXT SYMMETRY OPER *****  SEAR1290
      IF(NW(N)-NW(N-1))400,235,235                                      SEAR1300
  235 CONTINUE                                                          SEAR1310
C     ***** L CELL TRANSLATIONS IN X *****                              SEAR1320
      DO 395 L#LL,LU                                                    SEAR1330
      V(1)#U(1)+FLOATF(L-5)                                             SEAR1340
C     ***** M CELL TRANSLATIONS IN Y *****                              SEAR1350
      DO 395 M#ML,MU                                                    SEAR1360
      V(2)#U(2)+FLOATF(M-5)                                             SEAR1370
C     ***** N CELL TRANSLATIONS IN Z *****                              SEAR1380
      DO 395 NN#NL,NU                                                   SEAR1390
      V(3)#U(3)+FLOATF(NN-5)                                            SEAR1400
C     ***** I # TARGET ATOM *****                                       SEAR1410
      DO 395 I#ITAR1,ITAR2                                              SEAR1420
      DO 250 J#1,3                                                      SEAR1430
      TEM#0.0                                                           SEAR1440
      DO 245 II#1,3                                                     SEAR1450
  245 TEM#TEM+FS(II,J,K)*P(II,I)                                        SEAR1460
C     ***** SEE IF WITHIN PARALLELEPIPED*****                           SEAR1470
      TEM#TEM-V(J)                                                      SEAR1480
      IF(DX(J)-TEM)395,395,250                                          SEAR1490
  250 X(J)#TEM                                                          SEAR1500
      IF(KFUN-403)255,252,255                                           SEAR1510
C     ***** SEE IF WITHIN MODEL BOX *****                               SEAR1520
  252 CALL VM(X,AAREV,VI(2))                                            SEAR1530
      DO 253 J#2,4                                                      SEAR1540
      IF(AIN(J+3)-ABSF(VI(J)))395,253,253                               SEAR1550
  253 CONTINUE                                                          SEAR1560
      GO TO 277                                                         SEAR1570
C     ***** SEE IF WITHIN SPHERE *****                                  SEAR1580
  255 DSQ#VMV(X,AA,X)                                                   SEAR1590
      IF(DMX-DSQ)395,256,256                                            SEAR1600
  256 IF(DSQ-.0001)258,260,260                                          SEAR1610
  258 IF(KFUN-402)395,260,395                                           SEAR1620
C     ***** SELECT VECTORS ACCORDING TO CODES IF ANY *****              SEAR1630
  260 TEM#SQRTF(DSQ)                                                    SEAR1640
      IF(NCD)277,277,268                                                SEAR1650
  268 DO 275 J#1,NCD                                                    SEAR1660
  269 IF(ITOM-KD(1,J))275,270,270                                       SEAR1670
  270 IF(KD(2,J)-ITOM)275,271,271                                       SEAR1680
  271 IF(I-KD(3,J))   275,272,272                                       SEAR1690
  272 IF(KD(4,J)-I)   275,273,273                                       SEAR1700
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  273 IF(TEM-CD(1,J)) 275,274,274                                       SEAR1710
  274 IF(CD(2,J)-TEM) 275,277,277                                       SEAR1720
  275 CONTINUE                                                          SEAR1730
      GO TO 395                                                         SEAR1740
  277 VI(1) # 100000.*FLOATF(I)+FLOATF((1110-L*100-M*10-NN)*100+K)      SEAR1750
      IF(KFUN-402)278,325,325                                           SEAR1760
C     ***** DETERMINE CORRECT POSITION IN SORTED VECTOR TABLE *****     SEAR1770
  278 IF(NUM)317,317,279                                                SEAR1780
  279 DO 315 II#1,NUM                                                   SEAR1790
      TT#S(2,II)-TEM                                                    SEAR1800
      IF(ABSF(TT)-0.0001)297,297,281                                    SEAR1810
  281 IF(TT)315,297,283                                                 SEAR1820
C     ***** MOVE LONGER VECTORS TOWARD END OF TABLE *****               SEAR1830
  283 IF(200-NUM)287,287,289                                            SEAR1840
  287 NUM#199                                                           SEAR1850
  289 IJ#NUM                                                            SEAR1860
      DO 295 J#II,NUM                                                   SEAR1870
      S(1,IJ+1)#S(1,IJ)                                                 SEAR1880
      S(2,IJ+1)#S(2,IJ)                                                 SEAR1890
  295 IJ#IJ-1                                                           SEAR1900
      GO TO 319                                                         SEAR1910
C     ***** CHECK FOR DUPLICATE VECTORS IF DISTANCES ARE EQUAL *****    SEAR1920
  297 CALL ATOM(S(1,II),Z)                                              SEAR1930
      DO 305 J#1,3                                                      SEAR1940
      IF(ABSF(X(J)+Y(J)-Z(J))-0.0001)305,305,315                        SEAR1950
  305 CONTINUE                                                          SEAR1960
      GO TO 395                                                         SEAR1970
  315 CONTINUE                                                          SEAR1980
      IF(200-NUM)395,395,317                                            SEAR1990
C     ***** STORE THE RESULT IN VECTOR TABLE *****                      SEAR2000
  317 II#NUM+1                                                          SEAR2010
  319 NUM#NUM+1                                                         SEAR2020
      S(1,II)#VI(1)                                                     SEAR2030
      S(2,II)#TEM                                                       SEAR2040
      GO TO 395                                                         SEAR2050
C     ***** STORE RESULT IN ATOMS TABLE *****                           SEAR2060
  325 DO 330 J#1,3                                                      SEAR2070
  330 VI(J+1)#X(J)+Y(J)                                                 SEAR2080
      CALL STORE                                                        SEAR2090
  395 CONTINUE                                                          SEAR2100
  400 CONTINUE                                                          SEAR2110
C     ***** PRINT OUT DISTANCES *****                                   SEAR2120
  421 FORMAT(1H010X,20HVECTORS FROM ATOM  (I3,1H,I5,1H)6X,8HTO ATOMSI4, SEAR2130
     18H THROUGHI4)                                                     SEAR2140
      I0#SYITOM                                                         SEAR2150
      WRITE OUTPUT TAPE NOUT,421,ITOM,I0,ITAR1,ITAR2                    SEAR2160
      IF(NUM)500,500,423                                                SEAR2170
  423 DO 435 I#1,NUM                                                    SEAR2180
      T2#S(1,I)                                                         SEAR2190
      I1#T2/100000.                                                     SEAR2200
      I2#T2-FLOATF(I1)*100000.                                          SEAR2210
      CALL ATOM(T2,Z)                                                   SEAR2220
      IF(I-1)432,432,434                                                SEAR2230
  427 FORMAT(1H 13X,2(A6,1X),39X,1H(I3,1H,I5,1H)3F7.4,7X,3HD #F6.3)     SEAR2240
  429 FORMAT(1H 13X,2(A6,1X),2(3H  (I3,1H,I5,1H)3F7.4,3X)4X,3HD #F6.3)  SEAR2250
  432 WRITE OUTPUT TAPE NOUT,429,CHEM(ITOM),CHEM(I1),ITOM,I0,(Y(J),J#1,3SEAR2260
     1),I1,I2,(Z(J),J#1,3),S(2,I)                                       SEAR2270
      GO TO 435                                                         SEAR2280
  434 WRITE OUTPUT TAPE NOUT,427,CHEM(ITOM),CHEM(I1),I1,I2,(Z(J),J#1,3),SEAR2290
     1S(2,I)                                                            SEAR2300
  435 CONTINUE                                                          SEAR2310
C     ***** CALCULATE ANGLES ABOUT REF ATOM IF CODE IS 102 *****        SEAR2320
  437 IF(NJ2-2)500,451,451                                              SEAR2330
  441 FORMAT(1H010X,18HANGLES AROUND ATOMI5)                            SEAR2340
  451 WRITE OUTPUT TAPE NOUT,441,ITOM                                   SEAR2350
      L#NUM-1                                                           SEAR2360
      IF(L)500,500,457                                                  SEAR2370
  457 DO 465 I#1,L                                                      SEAR2380
      T2#S(1,I)                                                         SEAR2390
      T3#S(2,I)                                                         SEAR2400
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      I1#T2/100000.                                                     SEAR2410
      I2#T2-FLOATF(I1)*100000.                                          SEAR2420
      CALL ATOM(T2,X)                                                   SEAR2430
      CALL DIFV(X,Y,U)                                                  SEAR2440
      CALL MV(AA,U,V2)                                                  SEAR2450
      M#I+1                                                             SEAR2460
      DO 465 J#M,NUM                                                    SEAR2470
      T4#S(1,J)                                                         SEAR2480
      J1#T4/100000.                                                     SEAR2490
      J2#T4-FLOATF(J1)*100000.                                          SEAR2500
      CALL ATOM(T4,Z)                                                   SEAR2510
      CALL DIFV(Z,Y,V)                                                  SEAR2520
      F#ARCCOS(VV(V,V2)/(T3*S(2,J)))                                    SEAR2530
  460 FORMAT(1H 13X,3(A6,1X),7X,3(2H (I3,1H,I5,1H)),31X,F6.2)           SEAR2540
  465 WRITE OUTPUT TAPE NOUT,460,CHEM(I1),CHEM(ITOM),CHEM(J1),I1,I2,ITOMSEAR2550
     1,I0,J1,J2,F                                                       SEAR2560
  495 CONTINUE                                                          SEAR2570
  500 CONTINUE                                                          SEAR2580
  600 RETURN                                                            SEAR2590
      END                                                               SEAR2600
*LIST8
*LABEL
      SUBROUTINE SPARE(NJ)                                              SPAR0010
      COMMON NG                                                         SPAR0020
      NG#9                                                              SPAR0030
      RETURN                                                            SPAR0040
      END                                                               SPAR0050
*LIST8
*LABEL
      SUBROUTINE STORE                                                  STOR0010
C     ***** STORE IN OR REMOVE FROM ATOMS ARRAY *****                   STOR0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    STOR0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)STOR0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) STOR0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) STOR0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   STOR0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   STOR0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     STOR0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   STOR0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD STOR0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1STOR0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   STOR0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                STOR0140
      IF(LATM)481,481,450                                               STOR0150
  450 IF(500-LATM)455,455,460                                           STOR0160
  455 IF(NJ2-10)490,490,460                                             STOR0170
  460 L#LATM                                                            STOR0180
C     ***** CHECK FOR POSITIONAL DUPLICATION *****                      STOR0190
      DO 480 K#1,L                                                      STOR0200
      DO 465 J#2,4                                                      STOR0210
      IF(ABSF(V1(J)-ATOMS(J,K))-0.001)465,465,480                       STOR0220
  465 CONTINUE                                                          STOR0230
      IF(NJ2-10)490,490,470                                             STOR0240
C     ***** ATOM REMOVAL BY TABLE PUSHDOWN *****                        STOR0250
  470 LATM#LATM-1                                                       STOR0260
      DO 475 I#K,LATM                                                   STOR0270
      DO 475 J#1,4                                                      STOR0280
  475 ATOMS(J,I)#ATOMS(J,I+1)                                           STOR0290
      GO TO 490                                                         STOR0300
  480 CONTINUE                                                          STOR0310
  481 IF(NJ2-10)482,490,490                                             STOR0320
C     ***** STORE ATOM *****                                            STOR0330
  482 IF(499-LATM)490,483,485                                           STOR0340
  483 NG#16                                                             STOR0350
      CALL ERPNT (V1(1),400)                                            STOR0360
  485 LATM#LATM+1                                                       STOR0370
      DO 486 J#1,4                                                      STOR0380
  486 ATOMS(J,LATM)#V1(J)                                               STOR0390
  490 RETURN                                                            STOR0400
      END                                                               STOR0410
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*LIST8
*LABEL
      SUBROUTINE TMM(X,Y,Z)                                             TMM 0010
C     ***** TRANSPOSE(TRANSPOSE(X)*Y)#Z *****                           TMM 0020
C     ***** X,Y,Z ARE 3X3 MATRICES *****                                TMM 0030
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                    TMM 0040
      DO 115 I#1,3                                                      TMM 0050
      DO 115 K#1,3                                                      TMM 0060
  115 Z(K,I)#X(1,I)*Y(1,K)+X(2,I)*Y(2,K)+X(3,I)*Y(3,K)                  TMM 0070
      RETURN                                                            TMM 0080
      END                                                               TMM 0090
*LIST8
*LABEL
      SUBROUTINE UNIT(X,Z,ITYPE)                                        UNIT0010
      DIMENSION X(3),Y(3),Z(3)                                          UNIT0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    UNIT0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)UNIT0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) UNIT0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) UNIT0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   UNIT0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   UNIT0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     UNIT0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   UNIT0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD UNIT0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIUNIT0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   UNIT0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                UNIT0140
      Y(1)#X(1)                                                         UNIT0150
      Y(2)#X(2)                                                         UNIT0160
      Y(3)#X(3)                                                         UNIT0170
      IF(ITYPE)125,125,105                                              UNIT0180
  105 TI#SQRTF(Y(1)*Y(1)+Y(2)*Y(2)+Y(3)*Y(3))                           UNIT0190
      GO TO 145                                                         UNIT0200
  125 TI#SQRTF(Y(1)*(Y(1)*AA(1,1)+Y(2)*(AA(1,2)+AA(2,1))+Y(3)*(AA(1,3)+AUNIT0210
     1A(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2)))+Y(3)*Y(3)*AA(3UNIT0220
     2,3))                                                              UNIT0230
  145 IF(TI)155,155,175                                                 UNIT0240
  155 NG#5                                                              UNIT0250
      GO TO 300                                                         UNIT0260
  175 Z(1)#Y(1)/TI                                                      UNIT0270
      Z(2)#Y(2)/TI                                                      UNIT0280
      Z(3)#Y(3)/TI                                                      UNIT0290
  300 RETURN                                                            UNIT0300
      END                                                               UNIT0310
*LIST8
*LABEL
      SUBROUTINE VM(X,Y,Z)                                              VM  0010
C     TRANSPOSED VECTOR TIMES MATRIX                                    VM  0020
C     Z(3)#X(3)*Y(3,3)                                                  VM  0030
      DIMENSIONX(3),Y(3,3),Z(3)                                         VM  0040
      DO115J#1,3                                                        VM  0050
      Z(J)#0.0                                                          VM  0060
      DO115I#1,3                                                        VM  0070
  115 Z(J)#Z(J)+X(I)*Y(I,J)                                             VM  0080
      RETURN                                                            VM  0090
      END                                                               VM  0100
*LIST8
*LABEL
      FUNCTION VMV(X1,Q,X2)                                             VMV 0010
C     TRANSPOSED VECTOR * MATRIX * VECTOR                               VMV 0020
C     VMV#X1(3)*Q(3,3)*X2(3)    TO  EVALUATE QUADRATIC OR BILINEAR FORM VMV 0030
      DIMENSION X1(3),Q(3,3),X2(3)                                      VMV 0040
      TI#0.                                                             VMV 0050
      DO 10 J#1,3                                                       VMV 0060
   10 TI#TI+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))              VMV 0070
      VMV#TI                                                            VMV 0080
      RETURN                                                            VMV 0090
      END                                                               VMV 0100
*LIST8
*LABEL
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      FUNCTION VV(X,Y)                                                  VV   0010
C     TRANSPOSED VECTOR * VECTOR                                        VV   0020
C     VV#X(3)*Y(3)                                                      VV   0030
      DIMENSIONX(3),Y(3)                                                VV   0040
      VV#X(1)*Y(1)+X(2)*Y(2)+X(3)*Y(3)                                  VV   0050
      RETURN                                                            VV   0060
      END                                                               VV   0070
*LIST8
*LABEL
      SUBROUTINE XYZ(QA,X,ITYPE)                                        XYZ 0010
C     ***** ITYPE .GT.0 CART. COORD. FROM ATOM CODE WORD *****          XYZ 0020
C     ***** XABSF(ITYPE) .LE.2 FOR WORKING SYSTEM *****                 XYZ 0030
C     ***** XABSF(ITYPE) .GT.2 FOR REFERENCE SYSTEM *****               XYZ 0040
C     ***** ITYPE .LE.0 USES TRICLINIC COORD. XT *****                  XYZ 0050
      DIMENSION X(3)                                                    XYZ 0060
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    XYZ 0070
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)XYZ 0080
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) XYZ 0090
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) XYZ 0100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   XYZ 0110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   XYZ 0120
      DIMENSION XLNG(3),XO(3),XT(3)                                     XYZ 0130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   XYZ 0140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD XYZ 0150
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIXYZ 0160
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   XYZ 0170
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                XYZ 0180
      IT#XABSF(ITYPE)-2                                                 XYZ 0190
      NGI#NG                                                            XYZ 0200
      NG#0                                                              XYZ 0210
      IF(ITYPE)10,10,5                                                  XYZ 0220
    5 CALL ATOM(QA,XT)                                                  XYZ 0230
      IF(NG)30,10,30                                                    XYZ 0240
   10 T1#0.                                                             XYZ 0250
      DO 15 J#1,3                                                       XYZ 0260
      T2#XT(J)-ORGN(J)                                                  XYZ 0270
      V1(J)#T2                                                          XYZ 0280
   15 T1#T1+ABSF(T2)                                                    XYZ 0290
      IF(T1-.0001)20,20,40                                              XYZ 0300
   20 NG#NGI                                                            XYZ 0310
   30 DO 35 J#1,3                                                       XYZ 0320
   35 X(J)#0.                                                           XYZ 0330
      GO TO 300                                                         XYZ 0340
   40 IF(IT)45,45,60                                                    XYZ 0350
C     ***** RELATIVE TO WORKING SYSTEM *****                            XYZ 0360
   45 DO 55 I#1,3                                                       XYZ 0370
      T1#0.                                                             XYZ 0380
      DO 50 J#1,3                                                       XYZ 0390
   50 T1#T1+V1(J)*AAWRK(J,I)                                            XYZ 0400
   55 X(I)#T1*SCALI                                                     XYZ 0410
      GO TO 300                                                         XYZ 0420
C     ***** RELATIVE TO REFERENCE SYSTEM *****                          XYZ 0430
   60 DO 70 I#1,3                                                       XYZ 0440
      T1#0.                                                             XYZ 0450
      DO 65 J#1,3                                                       XYZ 0460
   65 T1#T1+V1(J)*AAREV(J,I)                                            XYZ 0470
   70 X(I)#T1*SCALI                                                     XYZ 0480
  300 RETURN                                                            XYZ 0490
      END                                                               XYZ 0500
```

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Carroll K. Johnson

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CHEMISTRY DIVISION

OR TEP-II:
A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Carroll K. Johnson

Revised February 1976

MARCH 1976

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OR TEP II: A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Carroll K. Johnson

ABSTRACT

This report describes a computer program for drawing crystal structure illustrations with a mechanical plotter. Ball-and-stick type illustrations of a quality suitable for publication are produced with either spheres or thermal-motion probability ellipsoids on the atomic sites. The program can produce stereoscopic pairs of illustrations which aid in the visualization of complex packing arrangements of atoms and thermal motion patterns. Interatomic distances, bond angles, and principal axes of thermal motion are also calculated to aid the structural study.

The most recent version of the program, OR TEP-II, has a hidden-line-elimination feature to omit those portions of atoms or bonds behind other atoms or bonds.

1. INTRODUCTION

Appropriate illustrations are essential in any manuscript dealing with crystallographic structures. An often quoted expression might justifiably be paraphrased to read that a well-planned figure is worth a thousand numbers. With the so-called information explosion in the scientific literature, the author of a structure paper should feel particularly obligated to help the reader as much as he can with "crystal clear" illustrations.

This computer program, OR TEP (Oak Ridge Thermal-Ellipsoid Plot program) is an attempt to supply a tool which can reduce the tedium associated with drawing certain types of crystal structure illustrations. In addition, the precision obtainable through machine plotting makes feasible the production of detailed stereoscopic illustrations which are impractical to draw by conventional drafting methods. The program does not in any sense replace the experience of the crystallographic draftsman; it is only a way of implementing certain of his ideas. Touching up the figures by hand, to add further detail, often enhances the figure's appeal and usefulness. The user is encouraged to do this and not to be content with the raw illustrations as they come from the plotter.

Four major goals were specified for OR TEP, and they are listed here in the order of their assigned importance. (1) The program must produce high quality illustrations, including stereoscopic pairs of thermal-motion figures, as free as possible of visually distracting approximations. (2) The program must be general both with respect to the types of illustrations it can draw and the types of computing and plotting equipment that it can utilize. (3) The program must be easy to use, require a minimum of input, and be easy to modify. (4) The computation time should be minimized. Memory size limitation was not of the considerations; hence the program requires at least a 32 K word memory.

Stereoscopic crystal structure illustrations were used quite extensively in the 1920's and 1930's, particularly by M. von Laue and R. von Mises in their beautifully done two-volume series of stereoscopic drawings.[1] More recently, computer techniques were applied in making crystal structure stereoscopic pictures by W. R. Busing[2] using an IBM 704 computer with cathode ray tube output. The availability of larger, faster computers and higher resolution plotting devices led quite naturally to the present work. As usual, there is an unlimited horizon for future work with more sophisticated ideas and equipment.

I am particularly indebted to my colleagues, Drs. H. A. Levy, W. R. Busing, G. M. Brown, and R. D. Ellison, for many helpful discussions, and to R. A. Hollister, a summer participant with the ORNL Mathematics Division, who helped plan and code several parts of the program. The initial version of OR TEP was written as a subroutine for the Busing, Martin, and Levy Function and Error Program, OR FFE;[3] and many of the concepts and several of the subroutines of OR FFE are incorporated into the present program. Several parts of EIGEN were taken from a program written by R. E. Funderlic and B. Franz from the Central Data Processing group. Subroutine AXEQB was adapted from a subroutine obtained from the Oak Ridge Central Data Processing Library.

This report covers the following topics. First, Sect. 2.1 is a summary table of instructions and is the part of the report to which the experienced user will routinely refer. Next, the philosophy of the program is outlined and an example given. Section 3 defines the terms used in this report and describes the input in detail. The computational procedures used by the program are discussed in Sect. 4, and steps are outlined for adapting the program to other configurations of equipment. The next section summarizes the mathematics of thermal-motion probability ellipsoids. Section 6 contains a number of examples of figures produced with OR TEP. Most of these drawings are stereoscopic pairs of perspective projections and are included to illustrate the information transfer advantages gained through the use of stereo figures. The final section contains the complete OR TEP-II FORTRAN IV listing for the IBM 360.

2. GENERAL PRINCIPLES AND PROCEDURES

2.1 Summary Table of Instructions

A brief summary of the input cards is given at this point to serve as a check list for use with OR TEP. All aspects are explained in detail in Sect. 3.

1. *Title card* (see 3.2.1)
2. *Cell parameter card* (see 3.2.2)
3. *Symmetry cards* with sentinel in column 1 on last card (see 3.2.3)
4. *Atomic parameter cards* (two per atom) with sentinel in column 1 of very last card (see 3.2.4)
5. *Instruction cards* with -1 in columns 8 and 9 of final instruction card. The instructions are summarized in Table 2.1 and explained in detail in Sect. 3.3.

---

[1] M. von Laue and R. von Mises (eds.), *Stereoscopic Drawings of Crystal Structures*, vols. I and II, Springer, Berlin, 1926 and 1936.

[2] W. R. Busing, *Abstract of Washington, D.C., Meeting of the ACA, Jan. 24–27, 1960*, F-7, p. 23.

[3] W. R. Busing, K. O. Martin, and H. A. Levy, *OR FFE, a FORTRAN Crystallographic Function and Error Program*, ORNL-TM-306 (March 1964).

Table 2.1. Summary table of all instructions

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Structure analysis									
Distances	0 or 2	101	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Dist. + ang.	0 or 2	102	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Princ. axes	–	103	–	–	–	–	–	–	–
Dist. single convolute	–	105	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Dist. reiterate convolute	–	106	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Plotter control									
Initialize	–	201	–	–	–	–	–	–	–
Advance and term.	–	202	X(IN)	Y(IN)	–	–	–	–	–
Initialize CRT	–	203	XORG	YORG	IZORG				
Change CRT intensity	–	204	IZ-IZORG						
Plot boundary									
Dimensions	–	301	X(IN)	Y(IN)	VIEW(IN)	BRDR(IN)	–	–	–
Title rotation	–	302	THETA(°)	–	–	–	–	–	–
Retrace displace	–	303	X(IN)	–	–	–	–	–	–
Atoms list									
Run add	–	401	FROM (1)	(–) TO (1)	FROM (2)	(–) TO (2)	FROM (3)	(–) TO (3)	. . .
Run subtract	–	411	FROM (1)	(–) TO (1)	FROM (2)	(–) TO (2)	FROM (3)	(–) TO (3)	. . .
Sphere add	0 or 2	402	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Sphere subtract	0 or 2	412	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Box add	–	403	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Box subtract	–	413	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Triclinic box add	–	404	ORG 1	ORG 2	TAR 1	TAR 2	A/2	B/2	C/2
Triclinic box subtract	–	414	ORG 1	ORG 2	TAR 1	TAR 2	A/2	B/2	C/2
Convolute add	–	405	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Convolute subtract	–	415	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Reiterate convolute add	–	406	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Reiterate convolute subt.	–	416	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Zero atoms list	–	410	–	–	–	–	–	–	–
Cartesian system									
Definition	–	501	ORGN	V1A	V1B	V2A	V2B	–	–
Rotate reference	–	502	Axis No.	Rotate (°)	Axis No.	Rotate (°)	. . .	. . .	. . .
Rotate working	–	503	Axis No.	Rotate (°)	–	–	–	–	–
Translate working	–	504	ΔX (IN)	ΔY (IN)	ΔZ (IN)	–	–	–	–
Origin at centroid	–	505	–	–	–	–	–	–	–
Inertial axis system and origin at centroid	–	506	–	–	–	–	–	–	–
Store overlap data (Also see 822, 821)	0 or 2	511	0 –1 OVMRGN (IN)						

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Center and scale									
Explicit	–	601	XO (IN)	YO (IN)	SCAL1	SCAL2	–	–	–
Scale only	–	602	XO (IN)	YO (IN)	–	SCAL2	–	–	–
Center only	–	603	–	–	SCAL1	SCAL2	–	–	–
Center and scale	–	604	–	–	–	SCAL2	–	–	–
I.P. and I.S.[a]	–	611	ΔXO (IN)	ΔYO (IN)	ΔSCAL1	SCAL2	–	–	–
I.P. and scale	–	612	ΔXO (IN)	ΔYO (IN)	–	SCAL2	–	–	–
I.S. and center	–	613	–	–	ΔSCAL1	SCAL2	–	–	–
Ellipsoids									
Shaded football	0 or 1	701	–	–	–	–	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)	–	–	A0 (IN)	A1 (IN)	ANR (1)	ANR (2)	–	–	–
Football	0 or 1	702	(same as 701)						
Open model	0 or 1	703	(same as 701)						
Boundary only	0 or 1	704	(same as 701)						
Other types	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)	–	–	A0 (IN)	A1 (IN)	ANR (1)	ANR (2)			
As above except no	0 or 1	711	(same as 701)						
printed output of	0 or 1	712	(same as 701)						
individual coordinates	0 or 1	713	(same as 701)						
	0 or 1	714	(same as 701)						
	0 or 1	715	(same as 705)						
Bonds									
Explicit (cont.)	1 or 2	801	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	. . .
Implicit fancy (Format No. 2 trailer card)	2	802	–	–	–	–	–	–	–
Implicit line (Format No. 2 trailer card)	2	803	–	–	–	–	–	–	–
As above except	–	811	(same as 801)						
no printed output	2	812	(same as 802)						
	2	813	(same as 803)						
Bond overlap explicit	1 or 2	821	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	. . .
Bond overlap implicit	2	822	–	–	–	–	–	–	–
Labels									
Chem. Symb.	–	901	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Reg. titles. Format No. 3 title card	3	902	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Proj. Vect. title Format No. 3 title card	3	903	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Vector title Format No. 3 title card	3	913	ATOM-1	ATOM-2	–	–	HGT (IN)	PAR-OFF	PER-OFF

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Proj. bond label									
(1 dec. place)	–	904	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(2 dec. places)	–	905	(same as 904)						
(3 dec. places)	–	906	(same as 905)						
Bond label									
(1 dec. place)	–	914	ATOM-1	ATOM-2	–	–	HGT (IN)	PAR-OFF	PER-OFF
(2 dec. places)	–	915	(same as 914)						
(3 dec. places)	–	916	(same as 914)						
Centered symb. (pen up)	1	908	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(pen down)	1	909	(same as 908)						
(Format No. 1 trailer card)		–	SYMB#	–	–	–	–	–	–
Saved sequence	–								
Start	–	1101	–	–	–	–	–	–	–
Stop	–	1102	–	–	–	–	–	–	–
Execute	–	1103	–	–	–	–	–	–	–
Terminate job	–	–1	–	–	–	–	–	–	–
New job follows (from title card on)	–	–2	–	–	–	–	–	–	–

[a]I.P. and I.S. signifies increment position and increment scale.
[b]PAR-OFF signifies parallel offset (in.).
[c]PER-OFF signifies perpendicular offset (in.).

2.2 Programming a Nonstereoscopic Illustration for OR TEP

2.2.1 General Comments on Automated Graphics. – In order to produce high quality illustrations with OR TEP, one must in general use an iterative approach; that is, the illustration must usually be computed and plotted several times before an optimal figure is produced. With each trial, as many factors as possible are optimized to give a more informative and more esthetically pleasing result. One often requires about four trials for a stereoscopic figure of an unfamiliar structure (barring blunders and plotter malfunctions).

Overlap is one of the major problems, particularly for chemical symbols and bond distance labels. If the user is not drawing stereoscopic figures, it is often better to do the lettering with a LeRoy lettering template instead of the computer. The template lettering is neater than the computer lettering, and it can be positioned much more easily. However, for stereoscopic lettering the manual procedure appears to be unsatisfactory because of the necessity for exact relative placement of the lettering on the two views to maintain good stereopsis.

The major portions of the hidden line segments of atoms and bonds that are partially or totally behind other atoms and bonds may be omitted by using the overlap-elimination features of OR TEP-II. However, there are often areas where additional manual touch-up is needed. This can be accomplished by erasing or "whiting out" the remaining unwanted line segments. Even with stereo views, the features are more effective if overlap is taken care of, especially when "opaque" ellipsoids are used.

In order to maintain generality in OR TEP, the concept of programming is applied to the problem of drawing illustrations with a plotter. This concept allows access to a series of basic building block operations which are put together by the user to "program" an illustration. The instructions used in programming OR TEP are divided into the following categories: (1) instructions used to specify preliminary graphical details, (2) instructions used to compose an illustration, (3) instructions used to draw the illustration, (4) instructions used to repeat a sequence of other instructions, and (5) termination instructions. Each instruction starts on a separate punched card and contains an identifying number and whatever parameters are needed for the particular instruction. The general role of these instructions is explained in the remaining parts of Sect. 2, and the individual instructions are described in detail in Sect. 3.3. The simplest way to construct the program is, first, to scan through the list of instructions in numerical order and pick out the relevant ones to construct the framework of the program. Then certain other instructions are placed into the framework program to furnish the remaining "bookkeeping" details.

Let us assume that the structural data cards (described in 3.2) have been prepared for a crystal structure and that we want to prepare a program to draw a single nonstereographic figure of the contents of one unit cell. We describe next the general stepwise procedure one would follow to program such an illustration.

2.2.2 Preliminary Graphical Details. – The first instruction card should be the plotter control instruction 201 (see 3.3.3.1) which will initialize the plotting package.

Next, the plot boundary instruction 301 (see 3.3.4.1) is needed to set the following parameters: (1) X dimension in inches for the plot boundary, (2) Y dimension in inches for the plot boundary, (3) viewing

distance in inches for perspective projection (zero as a signal for parallel projection), and (4) border (or margin) dimension inside the boundary.

No other 200 or 300 series instructions are required for this particular hypothetical figure.

The preliminary graphical details are analogous to what a draftsman might do in setting up his drafting board in preparation for a drawing.

2.2.3 Composing the Illustration. – This step involves specifying: (1) which atoms are to be used as the figure subject, (2) the rotational orientation of the subject, and (3) the scaling and positioning of the subject relative to the drawing area. These three components of composition are implemented by the 400, 500, and 600 series instructions respectively.

For our hypothetical example, suppose we want to place the *b* crystal axis along the plotter *x* axis and the c axis of the crystal in the plotter *xy* plane as nearly as possible parallel to the plotter *y* axis. This setting can be accomplished with a 501 instruction (see 3.3.6.1) alone; but if additional reorientation were necessary, a 502 instruction (see 3.3.6.2) would also be used.

A triclinic box of enclosure can be described with a 404 instruction (see 3.3.5.4) to contain the desired atoms for the subject definition. The scaling and positioning of the subject to fill the drawing area may be accomplished automatically with a 604 instruction (see 3.3.7.1).

2.2.4 Drawing the Illustration. – Crystal structure illustrations of the ball-and-stick type are made up of three components: balls (atoms), sticks (bonds), and labels. The three components are drawn with the 700, 800, and 900 instruction series respectively; the first two instruction series can also perform certain types of labeling.

A new instruction 511 in the OR TEP-II version of the program was added to store information needed for the overlap correction. This instruction is used before the 700 and 800 series instructions.

The atom representation can be either a general ellipsoid or a boundary ellipse. In some cases these become a sphere and a circle. Chemical symbols may be plotted simultaneously with the atoms.

For our example we might simply draw circles and put the chemical symbols within the circles by using instruction 704 (see 3.3.8.1). This instruction will draw all the atoms of the subject and their chemical symbols.

The bonds are not always necessary in a drawing, but for structures with molecules or with distinctive groupings they are usually quite helpful. The most convenient method for describing and drawing bonds is instruction 812 (see 3.3.9.2). This instruction uses vector search codes (see 3.1.5) which reflect the user's knowledge of the structural chemistry and the interatomic distance ranges for the compound being drawn. Covalent bonds or any other desired type are found and drawn automatically from the list of atoms which make up the subject. If desired, the interatomic distance label can also be drawn with each bond (see 3.3.9).

Various types of labeling can be done with the 900 series instruction. The one which will most often be included is a caption for the figure, using instruction 902 (see 3.3.10.2).

2.2.5 Terminating the Drawing of the Illustration. – The plotter control instruction 202 (see 3.3.3.2) allows the user to remove the finished drawing from the plotting area and to place a fresh area of plot paper in position for any additional plots which may be drawn.

To terminate the computer job, a (−1) instruction (see 3.3.12) is used as the last instruction of the program.

2.3 Programming a Stereoscopic Illustration for OR TEP

A stereoscopic pair of figures is simply two perspective views of the subject as seen from two different viewpoints (which are usually about 6° apart). This pair is produced with OR TEP by programming for two drawings. A few additional instructions supplementary to those outlined in 2.2 are useful for producing stereo figures. These instructions are the stereoscopic rotation instruction 503 and the 1100 series of instructions, which facilitate the repetition of a series of instructions.

2.3.1 Stereoscopic Rotations. – In general, one member of a detailed stereoscopic illustration cannot be drawn completely independent of the other member of the pair because certain features (e.g., which octant of an ellipsoid is shaded) must be done identically in the two drawings. In OR TEP the "stereoscopically sensitive decisions" are handled by using two Cartesian coordinate systems: the reference Cartesian system and the working Cartesian system (see 3.1.8). The steps involved in picture composition (see 2.2.3) and the stereoscopically sensitive decisions are always based on the reference system, but the drawing of the illustration (see 2.2.4) is always based on the working system. A stereoscopic rotation is simply a rotation of the working system *from the reference system* about the axis which is vertical while viewing the final result. For example, a nominal rotation of +3° about the plotter *y* axis might be used for the left-eye view and a rotation of −3° about the same axis might be made before plotting the right-eye view, thus producing a total interocular angle of 6°.

A program to draw a stereo pair would involve the following steps:

1. preliminary graphical details,
2. composition of subject,
3. left-eye stereo rotation,
4. draw the subject,
5. advance the plotter,
6. right-eye stereo rotation,
7. draw the subject,
8. advance the plotter,
9. terminate the job.

2.3.2 Repeating a Sequence of Operations. – It should be noted that steps 7 and 8 in the stereo program of the last section are identical to steps 4 and 5. The program can be shortened somewhat by using the "saved sequence" instructions (see 3.3.11). A 1101 instruction (start saved sequence) would be placed between 3 and 4, and a 1102 instruction (end saved sequence) between 5 and 6. Then steps 7 and 8 can be replaced by a 1103 instruction (execute saved sequence).

Any sequence of instructions can be saved in this manner and repeated as many times as desired with 1103 instructions. For example, the saved sequence feature can be used to produce a complete series of views of a structure at (say) 15° intervals about an axis. Note that the instructions between the start and stop instructions are *both executed and saved* the first time through.

2.4 Drawing the Cubane Structure: An Example

The novel compound cubane[4] (C_4H_4) has been crystallized and the structure determined.[5] The carbon-carbon bonds lie along the edges of a cube within experimental error. The compound crystallizes with the trigonal symmetry of space group $R\bar{3}$. One carbon and one hydrogen are in special positions along the $\bar{3}$ axis, and the remaining carbon and hydrogen are in general positions. Anisotropic temperature factor coefficients were fitted to the carbon atoms during the least-squares refinement of the structure, and isotropic temperature factors were used for the hydrogen atoms.

The cell parameters are

$$a = b = c = 5.34 \text{ A},$$

$$\alpha = \beta = \gamma = 72.26^\circ.$$

The equivalent positions of space group[6] $R\bar{3}$ are $x,y,z;\ z,x,y;\ y,z,x;\ \bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};$ and $\bar{y},\bar{z},\bar{x}$.

The positional parameters for C1, C2, H1, and H2 are given as –0.18711, 0.19519, 0.10706; 0.11546, 0.11546, 0.11546; –0.3246, 0.3468, 0.1848; and 0.2100, 0.2100, 0.2100, respectively. The anisotropic temperature factors given for the carbon atoms are of the type called zero[7] in this report (see 3.2.4.2). The coefficients b_{11}, b_{22}, b_{33}, b_{12}, b_{13}; b_{23} for C1 and C2 are 0.0410, 0.0425, 0.0450, –0.0042, –0.0142, –0.0051; and 0.0468, 0.0468, 0.0468, –0.0143, –0.0143, –0.0143.

2.4.1 Data Input for Cubane

2.4.1.1 Title Card (see 3.2.1). – FORMAT (12A6)

Card No.

(1) CUBANE (E. B. FLEISCHER (1964) J. A. C. S. 86, 3889)

2.4.1.2 Cell Parameter Card (see 3.2.2). – FORMAT (6F9.6)

(2) 5.34 5.34 5.34 72.26 72.26 72.26

2.4.1.3 Symmetry Cards (see 3.2.3)

FORMAT (I1, F14.10, 3F3.0, 2(F15.10, 3F3.0))

(3) 0 0. 1 0 0 0. 0 1 0 0. 0 0 1

(4) 0 0. 0 0 1 0. 1 0 0 0. 0 1 0

---

[4] P. Eaton and T. Cole, *J. Am. Chem. Soc.* **86**, 3157 (1964).

[5] E. B. Fleischer, *J. Am. Chem. Soc.* **86**, 3889 (1964).

[6] N. F. M. Henry and K. Lonsdale (eds.), *International Tables for X-Ray Crystallography*, vol. I, Kynoch, Birmingham, 1962.

[7] Unfortunately, many authors of structure papers neglect to define the equation for the anisotropic temperature factor coefficients. In the present case, the type can be determined from the comparative isotropic temperature factor listed in anisotropic form in their Table I. In other instances one must arbitrarily choose a type (usually 0, 1, or 4 in the U.S.A.) and do the principal axis transformation, then check that the principal values are correct, or at least reasonable. In particular, the principal values must all be positive.

Card No.				
(5)	0	0. 0 1 0	0. 0 0 1	0. 1 0 0
(6)	0	0. −1 0 0	0. 0 −1 0	0. 0 0 −1
(7)	0	0. 0 0 −1	0. −1 0 0	0. 0 −1 0
(8)	1	0. 0 −1 0	0. 0 0 −1	0. −1 0 0

2.4.1.4 Atomic Parameter Cards. –

Positional parameters (see 3.2.4.1): FORMAT (A6, 3X, 5F9.6, F9.0)

Thermal parameters (see 3.2.4.2): FORMAT (11, F8.6, 5F9.6, F9.0)

Atoms 1 and 2 are entered with positional parameters type 0 and anisotropic temperature factors type 0.

Card No.								
(9)		C1				−.18711	.19519	.10706	0
(10)	0		.04100	.04250	.04500	−.00420	−.01420	−.00510	0
(11)		C2				.11546	.11546	.11546	0
(12)	0		.04680	.04680	.04680	−.01430	−.01430	−.01430	0

Atoms 3 and 4 are entered with positional parameters type 0 and with dummy sphere temperature factors (type 7) 0.1 A in radius.

(13)		H1				−.32460	.34680	.18480	0
(14)	0		.1						7
(15)		H2				.21000	.21000	.21000	0
(16)	0		.1						7

Atom 5 is a dummy atom at the cell origin with a blank card dummy sphere (see next to last paragraph of 3.2.4.2). This could also be entered with type 7 as were atoms 3 and 4.

(17)		ORGN				.00000	.00000	.00000	0
(18)	1								0

In the card deck for this sample program, extensive use of Format No. 3 trailer cards (see 3.3.1.4) is made as a method of including a comment with an instruction. This convention is not mandatory, but it is a convenient method for annotating a program. This example uses a wide range of instructions in order to demonstrate them. As in the case with any programming system, there are many ways of doing any given problem. The Formats are described in Sect. 3.3.

2.4.2 Analysis of Structure (see 3.3.2). – These instructions are not connected with producing the figure. They are shown here just to demonstrate how they are used. A 101 instruction is used to obtain a tabulation of the atoms surrounding one atom or a series of several designated atoms. To obtain a list of all atoms (hydrogen and carbon atoms) out to a limit of (say) 3.61 A about the two carbons C1 and C2, one would use the following instruction. (The notation is explained in Sect. 3.3.2.)

Card No.

(19) 101 155501 2 1 4 3.61

Atoms 1 through 2 of symmetry operation 1 — Atoms 1 through 4 of all symmetry and translation operations — *D* max

A 102 instruction gives both interatomic distances and interatomic angles. In order to find all covalent bonds and bond angles about the two carbons we might use the following instruction.

(20) 102 155501 2 1 4 1.8

In this case a smaller *D* max was used so that only the distances and angles of immediate interest would be computed.

2.4.3 Programming the Cubane Illustration. – First we must initialize the plotter package.

(21) 201

The two plot boundary dimensions can be equal for the present illustration since the cubane molecule is a cube. Suppose we use an 11- by 11-in. boundary and specify a 1.5-in. margin to give a total working area of 9 by 9 in. A 30-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 30 1.5

In general we would use retracing to make the lettering, and certain other details, stand out more prominently. However, for the test example we will eliminate the retracing so that the illustration will plot as fast as possible.

(23) 303 0

The subject of the illustration is a single cubane molecule, which we will now define. One way of designating this subject is to specify a sphere of enclosure, centered on the dummy atom 555501, which is at the center of a cubane molecule. A radius of 3.2 A should be adequate to isolate a single molecule.

Card No.

(24) 402 555501 5 (a) 1 4 (b) 3.2 (c)

where the several parts designate:

(*a*) a run of origin atom (center of sphere) from atom 5 to atom 5 in symmetry position 55501 (that is, in this example, a single sphere),

(*b*) a run of target atom from atom 1 to atom 4, and

(c) a sphere radius of 3.2 A.

To orient the molecule, we will first define a coordinate system along the edges of the cubane cube. We will then rotate the molecule relative to this coordinate system to minimize overlap.

The origin of the coordinate system will be positioned on the dummy atom No. 5. The desired coordinate system orientation will be defined by specifying two vectors from the special position atom 255501 to the two symmetry-related general-position atoms 155501 and 155502.

(25) 501 555501 255501 155501 255501 155502 0 0

A rotation of 25° about the *Y* axis (axis 2) followed by a rotation of 28° about the *X* axis (axis 1) will produce a satisfactory view of the molecule.

(26) 502 2 25 1 28

To scale and position the subject for projection onto the drawing board and to utilize all available space, we will use the 604 instruction, which will automatically set X0, Y0, and SCAL1. However, the ellipsoid scale factor ratio SCAL2 must be specified independently. If we want thermal ellipsoids corresponding to 50% probability, then we will enter 1.54 for SCAL2.

(27) 604 0 0 0 1.54

This completes the composition of the illustration.

The stereoscopic rotation for the left eye can be done at this point. We will use a rotation of 2.7° about the *Y* axis (axis 2) for the left-eye view. Later in the program, we will make a −2.7° rotation about the same axis for the right-eye view to give a total interocular angle of 5.4°.

(28) 503 2 2.7

Since the structure will be drawn twice, once for each eye, the "saved sequence" feature can be used to shorten the program. Note that the instructions between the start

Card No.

and stop instructions are both *executed and saved* the first time through. They can then be re-executed as many times as desired by using the "execute saved sequence" instruction 1103.

The 1101 instruction starts the saved sequence.

(29)		1101								

The 511 instruction stores the information needed for the overlap hidden-line correction (i.e., as projected boundary ellipses for each atom in the ATOMS list and a quadrangle approximation for each bond). The bonds are specified with a format No. 2 trailer card identical to that used in the 812 instruction described below.

(30)	2	511			0					
(31)		0	1	4	1	4	4	0.9	1.6	.04

The ATOMS list currently contains all the atom designators for one cubane molecule. We want to draw the molecule in two separate steps so that the hydrogen and carbon atoms can be given different graphical representations. To draw the carbon atoms (ANR = 1,2), we will construct a special code that (a) draws the three principal-plane forward traces and the boundary-plane trace (NPLANE = 4), (b) omits the reverse sides of the principal planes (NDOT = 0), (c) draws the forward principal axes without additional shading (NLINE = 1), and (d) omits the reverse principal axes (NDASH = 0). In addition we want the chemical symbols to be drawn with letters 0.2-in. high (before projection) and displaced from the atomic center by 0.6 in. in the horizontal direction and 0.7 in. in the vertical direction.

(32)	1	715		4	0	1	0	.2	.6	.7
(33)		0		0	0	1	2			

The 715 instruction is used, rather than 705, to shorten the output listing of the example. Normally we would use the 705 to obtain a listing of all coordinates.

Since the hydrogen atoms (ANR = 3, 4) are to be drawn with a standard model, the construction details will be taken care of automatically. We want chemical symbols 0.2 in. high and offset 0.35 in. horizontally and 0.4 in. vertically.

(34)	1	712		0	0	0	0	.2	.35	.4
(35)		0		0	0	3	4			

The most convenient procedure for drawing bonds is to use the implicit bond instruction 812. All other information can be entered with a single format No. 2 trailer card (vector search code card).

Card No.

(36) 2 812

(37) 0 $\underbrace{1 \quad 4}_{(a)}$ $\underbrace{1 \quad 4}_{(b)}$ $\underbrace{4}_{(c)}$ $\underbrace{.9 \quad 1.6}_{(d)}$ $\underbrace{.04}_{(e)}$

where

(*a*) and (*b*) are atom number runs for atom-pair bonds to be drawn,

(*c*) denotes bond type 4,

(*d*) denotes the distance range 0.9 to 1.6 A, which will cover all covalent bond distances, and

(*e*) the bond radius, is 0.04 A.

The remaining fields in the card can be blank, since a complete set of bond distance labels is not desired.

Because of the symmetry, there are only two different C – C bond lengths in cubane. These are C1-C1 and C1-C2. We shall label one example of each of these bonds. For variety let us label one with a normal bond-length label and the other with a perspective label. The two bonds which can be labeled most advantageously are (*a*) 155504 → 155503 and (*b*) 255504 → 155505. The labels will be 0.15 in. in height and displaced vertically from the bond center by – 0.4 in.

(38)	906	155504	155503	0	0	.15	0	–.4
(39)	916	255504	155505	0	0	.15	0	–.4

The final feature to be drawn is a caption (CUBANE) for the illustration. This can conveniently be positioned by "hanging" it from the dummy atom 555501 and "bouncing" it 1 in. off the lower *y* boundary.

(40)	3	902	555501	0	0	1.	.25	0	0

(41) CUBANE

The saved sequence can now be terminated.

(42) 1102

The plotter is then advanced 9 in. along x in preparation for the right-eye view.

(43) 202 9

The stereo rotation of –2.7° about axis 2 is now performed in preparation for the right-eye view. (Note that this rotation starts with the reference orientation, not the previous working orientation.)

(44) 503 2 –2.7

Card No.

The saved sequence can now be repeated for the right eye. Note that the atom list now contains the same information that it did when the first view was drawn.

(45) 1103

The illustration is now complete. The plotter is next advanced 20 in. along x to remove this figure from the working area.

(46) 202 20

A dummy plot for the CalComp system is now added to aid in stopping the CalComp plotter.

(47) 202 0

Finally we terminate the job and exit from the program.

(48) −1

2.4.4 Stereoscopic Illustration of the Examples. – Figure 2.1 shows the stereoscopic pair exactly as it was plotted by a mechanical CalComp system, except for photographic reduction. Figure 2.2 shows one-half of the same illustration at a larger scale. These drawings have not been retouched.

Note that one bond distance label was drawn in perspective along the bond, and the other was drawn as a regular label parallel to the page.

Figure 2.3 is an example of a figure without photographic reduction drawn by a CalComp plotter which has 0.005 in. step-size resolution. Another representation of the same structure is shown in Fig. 6.19.

The input data and OR TEP instructions for Fig. 2.3 are listed in 2.4.5.2. The user should examine this example carefully since several useful techniques are illustrated.

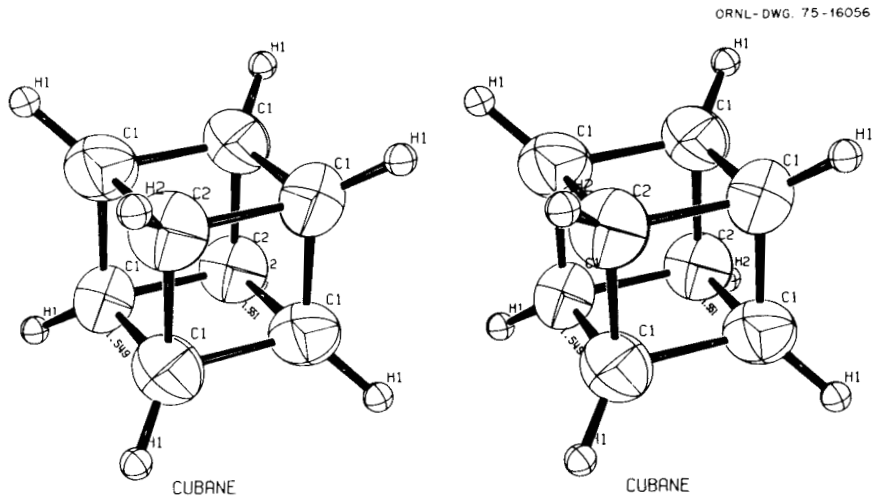

Fig. 2.1. The Sample Figure Cubane Reduced for Stereoscopic Viewing.

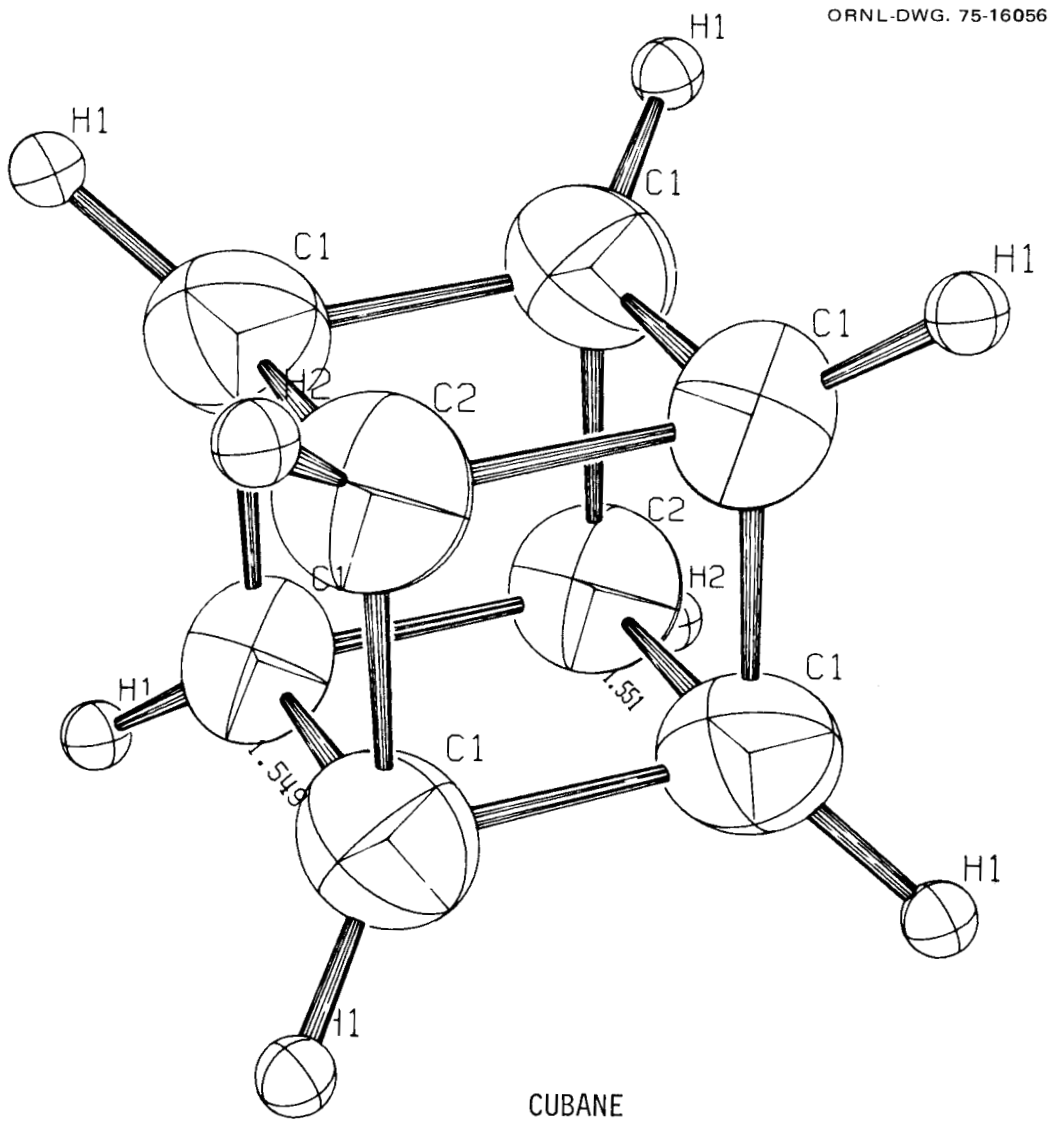

Fig. 2.2. The Sample Figure Cubane at 82% of Original Scale.

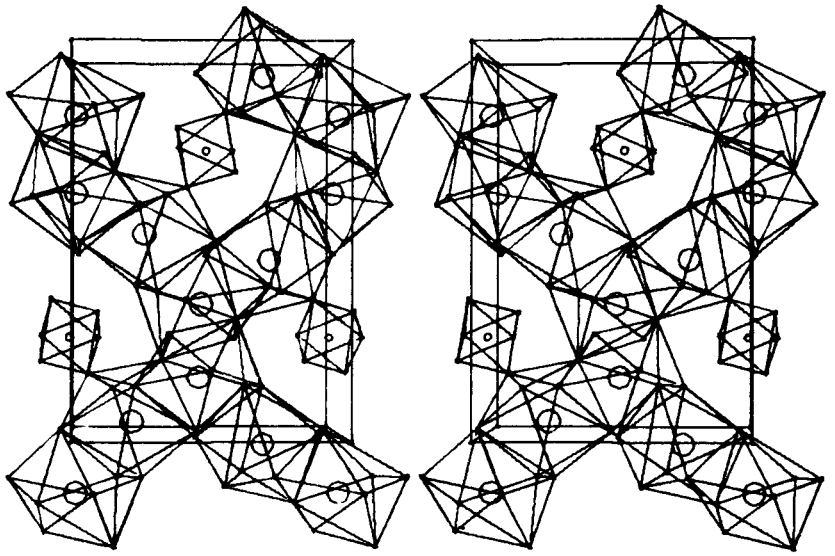

Fig. 2.3 Polyhedra Representation of Potassium Perxenate 9-Hydrate.

2.4.5 Listing of Sample Input and Output. – *2.4.5.1 Listing of Input Cards for Cubane.* –

```
 CUBANE  E.B.FLEISCHER    1964  J.A.C.S.  86,3889                          EXAM  10
     5.34      5.34      5.34     72.26     72.26     72.26                 EXAM  20
               0  1  0  0                0  0  1  0                0  0  0  1EXAM  30
               0  0  0  1                0  1  0  0                0  0  1  0EXAM  40
               0  0  1  0                0  0  0  1                0  1  0  0EXAM  50
               0 -1  0  0                0  0 -1  0                0  0  0 -1EXAM  60
               0  0  0 -1                0 -1  0  0                0  0 -1  0EXAM  70
1              0  0 -1  0                0  0  0 -1                0 -1  0  0EXAM  80
  C1                            -.18711   .19519   .10706         0         EXAM  90
   .04100    .04250    .04500  -.00420  -.01420  -.00510         0         EXAM 100
  C2                             .11546   .11546   .11546         0         EXAM 110
   .04630    .04680    .04680  -.01430  -.01430  -.01430         0         EXAM 120
  H1                            -.32460   .34680   .18480         0         EXAM 130
      .10                                                         7         EXAM 140
  H2                             .21000   .21000   .21000         0         EXAM 150
      .10                                                         7         EXAM 160
 ORGN                                 0         0         0         0         EXAM 170
1                                                               0         EXAM 180
  3   101   155501        2        1        4     3.61                    EXAM 190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****         EXAM 200
  3   102   155501        2        1        4      1.8                    EXAM 210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****             EXAM 220
  3   201                                                                 EXAM 230
***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****     EXAM 240
  3   301      11.      11.      30.      1.5                             EXAM 250
***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****     EXAM 260
  3   303                                                                 EXAM 270
***** ELIMINATE ALL RETRACING *****                                        EXAM 280
  3   402   555501        5        1        4      3.2                    EXAM 290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****      EXAM 300
  3   501   555501   255501   155501   255501   155502                  0EXAM 310
***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****EXAM 320
  3   502        2      25.        1      28.                            EXAM 330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****         EXAM 340
  3   604        0        0        0     1.54                            EXAM 350
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **EXAM 360
  3   503        2      2.7                                              EXAM 370
```

```
***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****          EXAM 380
  3  1101                                                                EXAM 390
***** START SAVE SEQUENCE *****                                          EXAM 400
  2   511        0                                                       EXAM 410
  3        1  4  1  4  4   0.9   1.6   .04                               EXAM 420
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULTEXAM 430
  1   715        4        0        1        0      .20      .60      .70EXAM 440
  3                                 1        2                           EXAM 450
***** DRAW CARBON ATOM ELLIPSOIDS, ATCM NUMBER RUN 1-2 *****             EXAM 460
  1   712                                          .20      .35      .40EXAM 470
  3                                 3        4                           EXAM 480
***** DRAW HYDROGEN ATOM SPHERES, ATCM NUMBER RUN 3-4 *****              EXAM 490
  2   812                                                                EXAM 500
  3        1  4  1  4  4   0.9   1.6   .04                               EXAM 510
***** TYPE 4 BONDS .04 A MEAN RADIUS, ATCMS 1-4 TO ATOMS 1-4, 0.9-1.6 A EXAM 520
  3   906   155504   155503        0        C      .15        0      -.4EXAM 530
***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****   EXAM 540
  3   916   255504   155505        0        0      .15        0      -.4EXAM 550
***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****EXAM 560
  3   902   555501        0        0      1.0      .25        0        0EXAM 570
                                CUBANE                                   EXAM 580
  3  1102                                                                EXAM 590
***** END OF SAVE SEQUENCE *****                                         EXAM 600
  3   202        9.                                                      EXAM 610
***** ADVANCE PLOTTER 9 INCHES ALONG X *****                             EXAM 620
  3   503        2     -2.7                                              EXAM 630
***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****   EXAM 640
  3  1103                                                                EXAM 650
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****                 EXAM 660
  3   202       20.                                                      EXAM 670
***** ADVANCE PLOTTER 20 INCHES *****                                    EXAM 680
  3   202                                                                EXAM 690
***** ADD DUMMY PLOT TO MAGNETIC TAPE *****                              EXAM 700
       -1                                                                EXAM 710
```

2.4.5.2 Listing of Input Cards for Potassium Perxenate 9-Hydrate. –

```
 POTASSIUM PERXENATE 9-HYDRATE/A.ZALKIN ET AL /(1964) JACS 86,3569      EXAM0010
    9.049   10.924   15.606      90.      90.      90.                   EXAM0020
             .0  1  0  0            .0  0  1  0            .0  0  0  1EXAM0030
             .0 -1  0  0            .0  0 -1  0            .5  0  0  1EXAM0040
             .0 -1  0  0            .5  0  1  0            .0  0  0  1EXAM0050
 1           .0  1  0  0            .5  0 -1  0            .5  0  0  1EXAM0060
  XE                            .249     .988     .250                   EXAM0070
     .10                                                   7            EXAM0080
  K1                            .628     .987     .339                   EXAM0090
     .30                                                   7            EXAM0100
  K2                            .846     .238     .958                   EXAM0110
     .30                                                   7            EXAM0120
  K3                            .307     .227     .026                   EXAM0130
     .30                                                   7            EXAM0140
  K4                            .877     .989     .139                   EXAM0150
     .30                                                   7            EXAM0160
  C1                            .403     .101     .251                   EXAM0170
     .20                                                   7            EXAM0180
  C2                            .094     .878     .253                   EXAM0190
     .20                                                   7            EXAM0200
  C3                            .138     .096     .316                   EXAM0210
     .20                                                   7            EXAM0220
  O4                            .176     .058     .151                   EXAM0230
     .20                                                   7            EXAM0240
  C5                            .323     .918     .351                   EXAM0250
     .20                                                   7            EXAM0260
```

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  C6                                .360     .881     .188                    EXAM0270
      .20                                                          7          EXAM0280
  W1                                .654     .839     .190                    EXAM0290
      .20                                                          7          EXAM0300
  W2                                .850     .136     .297                    EXAM0310
      .20                                                          7          EXAM0320
  W3                                .873     .829     .369                    EXAM0330
      .20                                                          7          EXAM0340
  W4                                .692     .046     .506                    EXAM0350
      .20                                                          7          EXAM0360
  W5                                .997     .243     .111                    EXAM0370
      .20                                                          7          EXAM0380
  W6                                .967     .980     .972                    EXAM0390
      .20                                                          7          EXAM0400
  W7                                .376     .470     .002                    EXAM0410
      .20                                                          7          EXAM0420
  W8                                .493     .262     .886                    EXAM0430
      .20                                                          7          EXAM0440
  W9                                .606     .150     .124                    EXAM0450
      .20                                                          7          EXAM0460
 ORGN                               .250     .500     .400                    EXAM0470
      .10                                                          7          EXAM0480
                                    .000     .000     .000                    EXAM0490
1     .03                                                          7          EXAM0500
  3   102   155501   555501          1        20      3.55                    EXAM0510
***** DISTANCES,ANGLES AND EDGES OF XE AND K COORDINATION POLYHEDRA ****EXAM0520
  3   201                                                                    EXAM0530
***** INITIALIZE CALCOMP PLOT PACKAGE *****                                  EXAM0540
  3   301        10        11        12      3.85                            EXAM0550
***** 10-2*3.85 # 2.3 IN. DIAMETER PICTURES,12 IN. AWAY,DIRECT STEREO VUEXAM0560
  3   401  2255501 -2266601                                                  EXAM0570
***** STORE UNIT CELL CORNERS FOR CELL OUTLINE *****                         EXAM0580
  3   404        21        21         1         5       .13       .52      .57EXAM0590
***** STORE CENTRAL ATOMS OF POLYHEDRA ****                                  EXAM0600
  3   405         1         5         1        20      3.52                    EXAM0610
***** CONVOLUTE SPHERE OF ENCLOSURE WITH EACH CENTRAL ATOM *****             EXAM0620
  3   501  2155501  2155501  2156501  2155501  2155601                       1EXAM0630
***** B AXIS HORIZONTAL, C AXIS VERTICAL, VIEWED ALONG -A AXIS *****         EXAM0640
  3   604                                                                    EXAM0650
***** AUTOMATIC SCALE AND POSITION *****                                     EXAM0660
  3   503         2         3                                                EXAM0670
***** STEREO ROTATION FOR LEFT EYE VIEW *****                                EXAM0680
  3  1101                                                                    EXAM0690
***** START SAVED SEQUENCE *****                                             EXAM0700
  1   714                                                                    EXAM0710
  3                                   1         5                            EXAM0720
***** DRAW METAL ATOMS SELECTIVELY *****                                     EXAM0730
  2   813                                                                    EXAM0740
  2       22 22 22 22  1   9.0  11.0   .01                                   EXAM0750
  2       22 22 22 22  1  15.0  16.0   .01                                   EXAM0760
  2        6 11  6 11  3   2.5   2.8   .04    -1      1   1.8   1.9          EXAM0770
  2        6 19  6 19  1   2.6   4.4   .02    -2      2   2.6   3.1          EXAM0780
  2       10 20 10 20  1   2.6   4.7   .02    -3      3   2.7  3.52          EXAM0790
  2        9 20  9 20  1   2.6  4.58   .02    -4      4   2.7   3.3          EXAM0800
  3        7 20  7 20  1   2.6   4.6   .02    -5      5   2.7   3.2          EXAM0810
***** DRAW POLYHEDRA AND CELL OUTLINE *****                                  EXAM0820
  3  1102                                                                    EXAM0830
***** END SAVED SEQUENCE *****                                               EXAM0840
  3   202       2.4                                                          EXAM0850
***** ADVANCE PLOTTER FOR RIGHT EYE VIEW *****                               EXAM0860
  3   503         2        -3                                                EXAM0870
***** STEREO ROTATION FOR RIGHT EYE VIEW *****                               EXAM0880
  3  1103                                                                    EXAM0890
***** REPEAT SAVED SEQUENCE                                                  EXAM0900
  3   202        10                                                          EXAM0910
***** ADVANCE PLOTTER 10 IN. *****                                           EXAM0920
  3   202                                                                    EXAM0930
***** ADD DUMMY PLOT  ( STOP CALCOMP ON PLOT NO. 3 ) *****                   EXAM0940
       -1                                                                    EXAM0950
```

2.4.5.3 Listing of Output from the Monitor Output Tape of the Computer. –

CUBANE E.B.FLEISCHER 1964 J.A.C.S. 86,3889

DIRECT CELL PARAMETERS

A	B	C	ALPHA	BETA	GAMMA
5.339999	5.339999	5.339999	72.260	72.260	72.260
		COSINE	0.30469871	0.30469871	0.30469871

RECIPROCAL CELL PARAMETERS

A*	B*	C*	ALPHA*	BETA*	GAMMA*
0.202207	0.202207	0.202207	103.506	103.506	103.506
		COSINE	-0.23353952	-0.23353940	-0.23353940

SYMMETRY TRANSFORMATIONS

NO.		TRANSFORMED X		TRANSFORMED Y		TRANSFORMED Z	
1	0.0	1. X 0. Y 0. Z	0.0	0. X 1. Y 0. Z	0.0	0. X 0. Y 1. Z	
2	0.0	0. X 0. Y 1. Z	0.0	1. X 0. Y 0. Z	0.0	0. X 1. Y 0. Z	
3	0.0	0. X 1. Y 0. Z	0.0	0. X 0. Y 1. Z	0.0	1. X 0. Y 0. Z	
4	0.0	-1. X 0. Y 0. Z	0.0	0. X -1. Y 0. Z	0.0	0. X 0. Y -1. Z	
5	0.0	0. X 0. Y -1. Z	0.0	-1. X 0. Y 0. Z	0.0	0. X -1. Y 0. Z	
6	0.0	0. X -1. Y 0. Z	0.0	0. X 0. Y -1. Z	0.0	-1. X 0. Y 0. Z	

NO.	ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23	TYPE
1	C1	-0.187110	0.195190	0.107060	0.041000	0.042500	0.045000	-0.004200	-0.014200	-0.005100	0.
2	C2	0.115460	0.115460	0.115460	0.046800	0.046800	0.046800	-0.014300	-0.014300	-0.014300	0.
3	H1	-0.324600	0.346800	0.184800	0.100000	0.0	0.0	0.0	0.0	0.0	7.
4	H2	0.210000	0.210000	0.210000	0.100000	0.0	0.0	0.0	0.0	0.0	7.
5	ORGN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.

NO.	ATOM	X	Y	Z	RMSD 1	RMSD 2	RMSD 3
1	C1	-0.187110	0.195190	0.107060	0.204899	0.239856	0.255794
2	C2	0.115460	0.115460	0.115460	0.205704	0.247732	0.247732
3	H1	-0.324600	0.346800	0.184800	0.100000	0.100000	0.100000
4	H2	0.210000	0.210000	0.210000	0.100000	0.100000	0.100000
5	ORGN	0.0	0.0	0.0	0.100000	0.100000	0.100000

```
CUBANE  E.B.FLEISCHER   1964  J.A.C.S.  86,3889

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR          Y VECTOR          Z VECTOR
   0.1872659E 00  -0.5990840E-01  -0.4722326E-01          0.5339996E 01   0.9536743E-06   0.9536743E-06
   0.0             0.1966153E C0  -0.4722328E-01          0.1627090E 01   0.5086076E 01   0.9536743E-06
   0.0             0.0             0.2022068E 00          0.1627090E 01   0.1187799E 01   0.4945430E 01

((((( INSTRUCTION  101 )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.3610000E 01  0.0            0.0

***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****

       FROM ATOMS    TO ATOMS     WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE   (MIN  MAX)   (MIN  MAX)                          A        B        C

101  155501   255501   1   4                         3.610    0.0      0.0

VECTORS FROM ATOM  (  1,55501)      TO ATOMS   1 THROUGH   4
     C1     H1     (  1,55501)-0.1871 0.1952 0.1071     (  3,55501)-0.3246 0.3468 0.1848        D = 1.012
     C1     C1                                          (  1,55505)-0.1071 0.1871-0.1952        D = 1.549
     C1     C1                                          (  1,55506)-0.1952-0.1071 0.1871        D = 1.549
     C1     C2                                          (  2,55501)  0.1155 0.1155 0.1155        D = 1.552
     C1     C1                                          (  1,55502)  0.1071-0.1871 0.1952        D = 2.183
     C1     C1                                          (  1,55503)  0.1952 0.1071-0.1871        D = 2.183
     C1     C2                                          (  2,55504)-0.1155-0.1155-0.1155        D = 2.202
     C1     H1                                          (  3,55506)-0.3468-0.1848 0.3246        D = 2.282
     C1     H1                                          (  3,55505)-0.1848 0.3246-0.3468        D = 2.306
     C1     H2                                          (  4,55501)  0.2100 0.2100 0.2100        D = 2.376
     C1     C1                                          (  1,55504)  0.1871-0.1952-0.1071        D = 2.677
     C1     H1                                          (  3,55502)  0.1848-0.3246 0.3468        D = 3.052
     C1     H1                                          (  3,55503)  0.3468 0.1848-0.3246        D = 3.069
     C1     H2                                          (  4,45501)-0.7900 0.2100 0.2100        D = 3.077
     C1     H2                                          (  4,56504)-0.2100 0.7900-0.2100        D = 3.096
     C1     H2                                          (  4,55504)-0.2100-0.2100-0.2100        D = 3.175
     C1     H1                                          (  3,55605)-0.1848 0.3246 0.6532        D = 3.200
     C1     H1                                          (  3,45603)-0.6532 0.1848 0.6754        D = 3.284
     C1     H1                                          (  3,46504)-0.6754 0.6532-0.1848        D = 3.388
     C1     C2                                          (  2,56504)-0.1155 0.8845-0.1155        D = 3.609

VECTORS FROM ATOM  (  2,55501)      TO ATOMS   1 THROUGH   4
     C2     H2     (  2,55501) 0.1155 0.1155 0.1155     (  4,55501)  0.2100 0.2100 0.2100        D = 1.109
     C2     C1                                          (  1,55501)-0.1871 0.1952 0.1071        D = 1.552
     C2     C1                                          (  1,55502)  0.1071-0.1871 0.1952        D = 1.552
     C2     C1                                          (  1,55503)  0.1952 0.1071-0.1871        D = 1.552
     C2     C1                                          (  1,55504)  0.1871-0.1952-0.1071        D = 2.202
     C2     C1                                          (  1,55505)-0.1071 0.1871-0.1952        D = 2.202
     C2     C1                                          (  1,55506)-0.1952-0.1071 0.1871        D = 2.202
     C2     H1                                          (  3,55501)-0.3246 0.3468 0.1848        D = 2.273
     C2     H1                                          (  3,55502)  0.1848-0.3246 0.3468        D = 2.273
     C2     H1                                          (  3,55503)  0.3468 0.1848-0.3246        D = 2.273
     C2     C2                                          (  2,55504)-0.1155-0.1155-0.1155        D = 2.710
     C2     H1                                          (  3,55504)  0.3246-0.3468-0.1848        D = 3.091
     C2     H1                                          (  3,55505)-0.1848 0.3246-0.3468        D = 3.091
     C2     H1                                          (  3,55506)-0.3468-0.1848 0.3246        D = 3.091
     C2     H1                                          (  3,56504)  0.3246 0.6532-0.1848        D = 3.181
     C2     H1                                          (  3,55605)-0.1848 0.3246 0.6532        D = 3.181
     C2     H1                                          (  3,65506)  0.6532-0.1848 0.3246        D = 3.181
     C2     C1                                          (  1,56504)  0.1871 0.8048-0.1071        D = 3.609
     C2     C1                                          (  1,55605)-0.1071 0.1871 0.8048        D = 3.609
     C2     C1                                          (  1,65506)  0.8048-0.1071 0.1871        D = 3.609
```

```
((((( INSTRUCTION  102 )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.1799999E 01  0.0            0.0

***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****

        FROM ATOMS    TO ATOMS     WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE    (MIN  MAX)   (MIN  MAX)                          A        B        C

102  155501   255501   1   4                          1.800    0.0      0.0


VECTORS FROM ATOM  (  1,55501)       TO ATOMS   1 THROUGH   4
     C1     H1     (  1,55501) -0.1871 0.1952 0.1071     (  3,55501)-0.3246 0.3468 0.1848       D = 1.012
     C1     C1                                           (  1,55505) -0.1071 0.1871-0.1952       D = 1.549
     C1     C1                                           (  1,55506) -0.1952-0.1071 0.1871       D = 1.549
     C1     C2                                           (  2,55501) 0.1155 0.1155 0.1155       D = 1.552

ANGLES AROUND ATOM    1
     H1     C1     C1          (  3,55501) (  1,55501) (  1,55505)            D = 2.282       A =124.69
     H1     C1     C1          (  3,55501) (  1,55501) (  1,55506)            D = 2.306       A =127.16
     H1     C1     C2          (  3,55501) (  1,55501) (  2,55501)            D = 2.273       A =123.52
     C1     C1     C1          (  1,55505) (  1,55501) (  1,55506)            D = 2.183       A = 89.60
     C1     C1     C2          (  1,55505) (  1,55501) (  2,55501)            D = 2.202       A = 90.48
     C1     C1     C2          (  1,55506) (  1,55501) (  2,55501)            D = 2.202       A = 90.48

VECTORS FROM ATOM  (  2,55501)       TO ATOMS   1 THROUGH   4
     C2     H2     (  2,55501) 0.1155 0.1155 0.1155     (  4,55501) 0.2100 0.2100 0.2100       D = 1.109
     C2     C1                                           (  1,55501) -0.1871 0.1952 0.1071       D = 1.552
     C2     C1                                           (  1,55502) 0.1071-0.1871 0.1952       D = 1.552
     C2     C1                                           (  1,55503) 0.1952 0.1071-0.1871       D = 1.552

ANGLES AROUND ATOM    2
     H2     C2     C1          (  4,55501) (  2,55501) (  1,55501)            D = 2.376       A =125.66
     H2     C2     C1          (  4,55501) (  2,55501) (  1,55502)            D = 2.376       A =125.66
     H2     C2     C1          (  4,55501) (  2,55501) (  1,55503)            D = 2.376       A =125.66
     C1     C2     C1          (  1,55501) (  2,55501) (  1,55502)            D = 2.183       A = 89.44
     C1     C2     C1          (  1,55501) (  2,55501) (  1,55503)            D = 2.183       A = 89.44
     C1     C2     C1          (  1,55502) (  2,55501) (  1,55503)            D = 2.183       A = 89.44

((((( INSTRUCTION  201 )))))
 0.0            0.0            0.0            0.0            0.0            0.0            0.0

***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****

((((( INSTRUCTION  301 )))))
 0.1100000E 02  0.1100000E 02  0.3000000E 02  0.1500000E 01  0.0            0.0            0.0

***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****

PLOT LIMITS 11.00 BY 11.00 IN.  INCLUDING  1.50  IN. MARGIN
VIEW DISTANCE 30.000 INCHES
```

22

```
(((((  INSTRUCTION  303 )))))
      0.0          0.0          0.0          0.0          0.0          0.0          0.0

     ***** ELIMINATE ALL RETRACING *****

     RETRACE DISPLACEMENT = 0.0    INCH

(((((  INSTRUCTION  402 )))))
      0.5555010E 06  0.5000000E 01  0.1000000E 01  0.4000000E 01  0.3200000E 01  0.0          0.0

     ***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****

            FROM ATOMS    TO ATOMS     WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
     CODE   (MIN  MAX)   (MIN  MAX)                          A        B        C

     402  555501   555501   1   4                          3.200    0.0      0.0

     VECTORS FROM ATOM  (  5,55501)      TO ATOMS   1 THROUGH   4

     CONTENTS OF ATOMS ARRAY
            155501.   255501.   355501.   455501.   155502.   355502.   155503.   355503.   155504.   255504.
            355504.   455504.   155505.   355505.   155506.   355506.

(((((  INSTRUCTION  501 )))))
      0.5555010E 06  0.2555010E 06  0.1555010E 06  0.2555010E 06  0.1555020E 06  0.0          0.0

     ***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0          0.0          0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1950173E 00  -0.5332431E-01   0.3517698E-02          -0.5161572E 01   0.2128973E 00   0.1352190E 01
        0.5138889E-01   0.4031152E-02   0.1955263E 00          -0.2760968E 00   0.1350079E 01   0.5159129E 01
       -0.5414121E-02   0.1954785E 00  -0.5144400E-01          -0.1402325E 01   0.5145890E 01   0.2624693E 00

(((((  INSTRUCTION  502 )))))
      0.2000000E 01  0.2500000E 02  0.1000000E 01  0.2800000E 02  0.0          0.0          0.0

     ***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0          0.0          0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1752591E 00  -0.8727211E-01   0.5055124E-01          -0.4106512E 01  -0.1411451E 01   0.3108037E 01
        0.1292071E 00  -0.6943828E-01   0.1391812E 00           0.1930112E 01  -0.1057861E 01   0.4865296E 01
       -0.2664803E-01   0.1934117E 00   0.5262519E-01          -0.1160014E 01   0.4153644E 01   0.3149157E 01

(((((  INSTRUCTION  604 )))))
      0.0          0.0          0.0          0.1540000E 01  0.0          0.0          0.0

     ***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **

     ORIGIN POINT IN PLOTTER COORD.(  5.35 ,  5.75 ) IN.
     OVERALL SCALE = 1.960 INCH/ANGSTROM ELLIPSOID SCALE = 1.540
     VIEW DISTANCE 30.000 INCHES
```

```
((((( INSTRUCTION  503 )))))
     0.2000000E 01  0.2700000E 01  0.0            0.0            0.0            0.0            0.0

     ***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

     ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                  POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1726831E 00  -0.8727211E-01   0.5875095E-01          -0.3955544E 01  -0.1411451E 01   0.3298029E 01
        0.1356199E 00  -0.6943828E-01   0.1329401E 00           0.2157155E 01  -0.1057861E 01   0.4768971E 01
       -0.2413946E-01   0.1934117E 00   0.5382206E-01          -0.1010380E 01   0.4153644E 01   0.3200305E 01

((((( INSTRUCTION 1101 )))))
     0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** START SAVE SEQUENCE *****

((((( INSTRUCTION  511 )))))
     0.0            0.0            0.0            0.0            0.0            0.0            0.0
       1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

     ***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT

     OVERLAP MARGIN IS 0.042 INCH
     CONTENTS OF SORTED ATOMS ARRAY
            455504.   255504.   355504.   355506.   155504.   155506.   355505.   155505.   355502.   155502.
            155503.   155501.   355503.   355501.   255501.   455501.

     BOND SELECTION CODES

     (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
     (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
         1    4       1    4       4  0.90  1.60   0.040   0.0     0.0     0.0     0.0       0.
     FAULT NG = 14   455504.   800


     BOND OVERLAP ARRAY CONTAINS  19 BONDS (MAXIMUM IS 599)
     ATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE IN SORTED ATOMS ARRAY
              2005.     2006.     2008.     3005.     4006.     5010.     5011.     6010.     6012.     7008.
              8011.     8012.     9010.    10015.    11013.    11015.    12014.    12015.    15016.

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

     ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1752591E 00  -0.8727211E-01   0.5055124E-01          -0.4106512E 01  -0.1411451E 01   0.3108037E 01
        0.1292071E 00  -0.6943828E-01   0.1391812E 00           0.1930112E 01  -0.1057861E 01   0.4865296E 01
       -0.2664803E-01   0.1934117E 00   0.5262519E-01          -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  715 )))))
     0.4000000E 01  0.0            0.1000000E 01  0.0            0.2000000E 00  0.6000000E 00  0.7000000E 00
     0.0            0.0            0.1000000E 01  0.2000000E 01  0.0            0.0            0.0

     ***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
```

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```
((((( INSTRUCTION  712 )))))
      0.0            0.0            0.0            0.0            0.2000000E 00  0.3500000E 00  0.4000000E 00
      0.0            0.0            0.3000000E 01  0.4000000E 01  0.0            0.0            0.0

     ***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****

((((( INSTRUCTION  812 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0
        1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

     ***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A

     BOND SELECTION CODES

     (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
     (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
          1    4       1    4       4  0.90  1.60   0.040   0.0     0.0     0.0     0.0       0.
     FAULT NG = 14   455504.   800

((((( INSTRUCTION  906 )))))
      0.1555040E 06  0.1555030E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

     ***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****

((((( INSTRUCTION  916 )))))
      0.2555040E 06  0.1555050E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

     ***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****

((((( INSTRUCTION  902 )))))
      0.5555010E 06  0.0            0.0            0.1000000E 01  0.2500000E 00  0.0            0.0

                                      CUBANE

((((( INSTRUCTION 1102 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** END OF SAVE SEQUENCE *****

((((( INSTRUCTION  202 )))))
      0.9000000E 01  0.0            0.0            0.0            0.0            0.0            0.0

     ***** ADVANCE PLOTTER 9 INCHES ALONG X *****

((((( INSTRUCTION  503 )))))
      0.2000000E 01 -0.2700000E 01  0.0            0.0            0.0            0.0            0.0

     ***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

     ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1774457E 00  -0.8727211E-01   0.4223930E-01          -0.4248361E 01  -0.1411451E 01   0.2911142E 01
        0.1225073E 00  -0.6943828E-01   0.1451131E 00           0.1698782E 01  -0.1057861E 01   0.4950814E 01
       -0.2909743E-01   0.1934117E 00   0.5131147E-01          -0.1307071E 01   0.4153644E 01   0.3091016E 01
```

```
((((( INSTRUCTION 1103 )))))
 0.0          0.0          0.0          0.0          0.0          0.0          0.0

***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****

((((( INSTRUCTION  511 )))))
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
   1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT

OVERLAP MARGIN IS 0.042 INCH

CONTENTS OF SORTED ATOMS ARRAY
       455504.   355504.   255504.   355506.   155504.   155506.   355505.   355502.   155502.   155505.
       155503.   155501.   355503.   355501.   255501.   455501.

BOND SELECTION CODES

(SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
(  MIN   MAX )(  MIN   MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
     1     4       1     4       4  0.90  1.60   0.040   0.0     0.0     0.0     0.0       0.
FAULT NG = 14   455504.   800


BOND OVERLAP ARRAY CONTAINS  19 BONDS (MAXIMUM IS 599)
ATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE IN SORTED ATOMS ARRAY
         2005.     3005.     3006.     3010.     4006.     5009.     5011.     6009.     6012.     7010.
         8009.     9015.    10011.    10012.    11013.    11015.    12014.    12015.    15016.

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR         Y VECTOR         Z VECTOR
  -0.1752591E 00  -0.8727211E-01   0.5055124E-01          -0.4106512E 01  -0.1411451E 01   0.3108037E 01
   0.1292071E 00  -0.6943828E-01   0.1391812E 00           0.1930112E 01  -0.1057861E 01   0.4865296E 01
  -0.2664803E-01   0.1934117E 00   0.5262519E-01          -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  715 )))))
 0.4000000E 01  0.0            0.1000000E 01  0.0            0.2000000E 00  0.6000000E 00  0.7000000E 00
 0.0            0.0            0.1000000E 01  0.2000000E 01  0.0            0.0            0.0

***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
((((( INSTRUCTION  712 )))))
 0.0            0.0            0.0            0.0            0.2000000E 00  0.3500000E 00  0.4000000E 00
 0.0            0.0            0.3000000E 01  0.4000000E 01  0.0            0.0            0.0

***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****
```

```
((((( INSTRUCTION  812 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0
        1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

     ***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A

     BOND SELECTION CODES

     (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
     (  MIN   MAX )(  MIN   MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
         1     4       1     4       4  0.90   1.60   0.040   0.0     0.0     0.0     0.0       0.
     FAULT NG = 14   455504.   800


((((( INSTRUCTION  906 )))))
      0.1555040E 06  0.1555030E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

     ***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****

((((( INSTRUCTION  916 )))))
      0.2555040E 06  0.1555050E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

     ***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****

((((( INSTRUCTION  902 )))))
      0.5555010E 06  0.0            0.0            0.1000000E 01  0.2500000E 00  0.0            0.0

                                      CUBANE

((((( INSTRUCTION 1102 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** END OF SAVE SEQUENCE *****

((((( INSTRUCTION  202 )))))
      0.2000000E 02  0.0            0.0            0.0            0.0            0.0            0.0

     ***** ADVANCE PLOTTER 20 INCHES *****

((((( INSTRUCTION  202 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** ADD DUMMY PLOT TO MAGNETIC TAPE *****

((((( INSTRUCTION   -1 )))))
```

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3. DETAILED OPERATING INSTRUCTIONS

3.1 Definitions

Several conventions must be defined before the instructions can be explained.

3.1.1 Atom Designator Code (ADC) and Addressable Point. – In order to specify a particular atom in the crystal within a reasonable distance from the crystallographically defined origin, the following five-component atom designator code word (ADC) is used.

$$ADC = AN*10^5 + (TA + 5)*10^4 + (TB + 5)*10^3 + (TC + 5)*10^2 + SN,$$

where

AN = *ATOM NUMBER* ($0 \leqq AN \leqq NATOM \leqq 166$) = the sequential number of the atom in the input list of atoms in the asymmetric unit, which contains NATOM atoms. Atom zero is not in the input atom list but refers to the crystal origin point (0., 0., 0.).

TA,TB,TC = *crystal lattice translation digits* along cell edges **a**, **b**, and **c**. Each digit in ADC can range from 1 to 9; consequently, it is possible to move up to ±4 lattice translations in any direction from the origin cell 5,5,5.

SN = *symmetry operator number* ($0 \leqq SN \leqq NSYM \leqq 48$) = the numerical position of the symmetry operator in the input symmetry operator list which contains NSYM entries. Symmetry operator number zero is not in the input list but refers to an identity operator. However, the identity operation (corresponding to position *x, y, z*) must in general also be somewhere in the input symmetry operator list and is usually the first operator.

Example: An atom designation code of *3 475 02* refers to atom 3 moved through symmetry operation 2, then translated – 1 cell translation along **a**, +2 cell translations along **b**, and 0 cell translations along **c**.

An *addressable point* in the crystal is any point for which an atom designator code exists. In general, the addressable region is approximately a 9 × 9 × 9 block of unit cells.

3.1.2 Vector Designator Code (VDC). – A vector direction is specified by two atom designator codes. The vector direction is from the first to the second.

Example: 253704 263704 is a vector along the positive **a** direction of the crystal lattice.

3.1.3 Atom Designator Run (ADR). – A straight run sequence of atoms can be defined using two atom designator codes with a negative sign preceding the second of the two. The run hierarchy is: first, atom number AN; second, symmetry operation SN; third, **a** translation TA; fourth, **b** translation TB; and last, **c** translation TC.

Example: ADR (145502 – 245603) will generate the 8-atom run 145502, 245502, 145503, 245503, 145602, 245602, 145603, 245603.

3.1.4 Atom Number Run (ANR). – The Atom Number Run is a subset of the Atom Designator Run. In this case, only the atom number AN is allowed to change. Normally, an ANR is entered by using only the atom number (AN) values for the first and last members of the sequence without a minus sign.

Example: (1 4) will designate atoms 1, 2, 3, and 4 of the input list.

3.1.5 Vector Search Code (VSC). – A vector search code consists of two atom number runs and a distance range. It is used for finding interatomic distances which have a particular chemical significance, such as covalent and coordination bonds.

Example: Suppose that metal atoms are numbers 1 and 2 in the atom list and oxygen atoms are 6–12 and that the interatomic distance range between metals and oxygens is 1.9 A to 2.4 A. The metal-to-oxygen vectors can be specified by the vector search code (1 2) (6 12) (1.9 2.4). Several variations of this basic code are used in the program.

3.1.6 Sphere of Enclosure. – The sphere of enclosure specifies some or all of the atoms lying within a sphere of radius *D* max about a given "origin" atom without the necessity of delineating each atom individually. This "sphere of enclosure" is said to contain a *complete population* if all addressable atoms within the *D* max radius are included. If the sphere of enclosure contains only certain types of atoms which are derived from a group of sequential atoms in the input list, then the sphere is said to have a *partial population.* Finally, the population (complete or partial) of the sphere of enclosure can be screened as selectively as desired through the use of vector search codes (3.1.5), and the resulting content is called a *vector screened population.*

A sphere of enclosure can be centered on any addressable atom, but one should not use points in the outermost cells as centers because of the possibility of having nonaddressable points within the *D* max radius.

3.1.7 Box of Enclosure. – This is a parallelepiped which can be centered about any addressable point and assigned arbitrary orientation and dimensions. This "box of enclosure" can have a *complete population* or a *partial population* as described for the sphere of enclosure (3.1.6). However, vector screening is not allowed with the box of enclosure.

3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems. – Many of the OR TEP calculations use fractional coordinates based on the crystal axes **a**, **b**, and **c** (triclinic coordinate system); but other steps necessitate the introduction of orthonormal base vector triplets (Cartesian coordinate systems). Two Cartesian systems (reference and working) are utilized. The reference (major) system is used for all operations except plotting, where the working (minor) system is used. For a right-eye or left-eye stereo view, the working system is moved from the reference system by rotation about an axis of the reference system. However, certain decisions made while plotting must still be referred to the reference system to maintain accurate stereopsis. The user can define and orient the two Cartesian systems through the instructions of series 500. Until a 500-series instruction is given, a "standard Cartesian system" is utilized for both the reference and working systems. The orthonormal base vectors of the standard system are oriented as follows:

$$x \text{ axis along } \mathbf{a},$$
$$y \text{ axis along } (\mathbf{a} \times \mathbf{b}) \times \mathbf{a},$$
$$z \text{ axis along } (\mathbf{a} \times \mathbf{b}) = \mathbf{c}^*,$$

where **a**, **b**, and **c** are crystal axes and $\times$ denotes the outer vector product (cross product). The symbol $\mathbf{c}^*$ refers to a reciprocal axis.

3.1.9 Prime Parameters and Primer Constants. – In the process of mathematically describing an illustration to be machine drawn, many parameters must be used. The more basic among these parameters are called *Prime Parameters*. The values assigned to these prime parameters are often similar or identical from one problem to the next. The first thing OR TEP does is to call subroutine PRIME, which sets as many prime parameters as possible to reasonable, "in the ball park," *Primer Constants*. For example, the maximum plot dimensions (instruction 300 series) are set at 17.0 in. for x maximum and 11.0 in. for y maximum, and the overall scale for plotting (instruction 600 series) is set at 1.0 in./A. If the value assigned to a particular constant by the primer routine is satisfactory, the user does not have to reset this constant with OR TEP instructions.

3.2 Crystal Structure Data Input

3.2.1 Title Card. – FORMAT (12A6)

Columns	
1–72	Title consisting of any desired alphanumeric identification information. This will appear periodically in the output.

3.2.2 Cell Parameter Card. – FORMAT (6F9.6). Any one of the four following input alternatives may be used (no indicator is needed to specify which type).[1]

Columns	Type A	Type B	Type C	Type D
1–9	**a** (A)	**a** (A)	**a*** (A^{-1})	**a*** (A^{-1})
10–18	**b** (A)	**b** (A)	**b*** (A^{-1})	**b*** (A^{-1})
19–27	**c** (A)	**c** (A)	**c*** (A^{-1})	**c*** (A^{-1})
28–36	α (deg)	cos α	α^* (deg)	cos α^*
37–45	β (deg)	cos β	β^* (deg)	cos β^*
46–54	γ (deg)	cos γ	γ^* (deg)	cos γ^*

The parameters **a***, etc., refer to the reciprocal unit cell such that **a**·**a*** = 1. All four types will be printed out regardless of which type was used for input.

3.2.3 Symmetry Cards (1 ≦ NSYM ≦ 48). – FORMAT (I1,F14.10, 3F3.0,2(F15.10,3F3.0)). The card will be interpreted in one of two ways, depending on the numerical value of the number in columns 70–72. If that number is <5.0, the card is interpreted as a crystallographic symmetry operation; but if the number is ≧5.0, the card is interpreted as a general helix-screw symmetry operation[2] along the **c*** crystal axis

[1]The routine assumes that **a** ≧ 1.0 A, **a*** < 1.0 A^{-1}, α (or α^*) ≧ 1.0°, and $|\cos \alpha|$ (or $|\cos \alpha^*|$) < 1.0.

[2]The general helix-screw symmetry operation is not an allowed element of a crystallographic group, so that the molecular environment of the transformed unit will not in general be identical to that of the untransformed unit (unless the crystal is considered to be one dimensional). This input is simply an expedient for use in plotting helical polymer structure models with minimum input. In general it would be possible to produce the same results by specifying the *complete crystallographic asymmetric unit* and normal crystallographic symmetry transformations.

This input mode is only meaningful if the cell angles α and β are 90°, so that **c** lies along **c*** and the helix can continue uninterrupted from cell to cell along the **c** axis.

(third axis of the standard Cartesian system; see 3.1.8). The two symmetry types can be intermixed if desired.

Columns	(*a*) Crystallographic symmetry (70–72 $\leq$ 5)	(*b*) Helix symmetry (70–72 $\geq$ 5)
1	$\neq 0$ last card only	$\neq 0$ last card only
2–15	T_1	T_1
16–18	S_{11}	–
19–21	S_{12}	–
22–24	S_{13}	–
25–39	T_2	T_2
40–42	S_{21}	–
43–45	S_{22}	–
46–48	S_{23}	–
49–63	T_3	T_3
64–66	S_{31}	L
67–69	S_{32}	M
70–72	S_{33}	N

(*a*) Crystallographic symmetry[3]: Transformed triclinic coordinates (X_1, Y_1, Z_1) are obtained from input triclinic coordinates (X, Y, Z) by

$$X_1 = T_1 + S_{11} X + S_{12} Y + S_{13} Z ,$$
$$Y_1 = T_2 + S_{21} X + S_{22} Y + S_{23} Z ,$$
$$Z_1 = T_3 + S_{31} X + S_{32} Y + S_{33} Z ,$$

or in matrix notation

$$\mathbf{X}_1 = \mathbf{T} + \mathbf{S}\,\mathbf{X} ,$$

where

$\mathbf{T} = (T_1, T_2, T_3)$ as fractions of cell edges.

(*b*) Helix screw symmetry:

$$\mathbf{X}_1 = \mathbf{T} + \mathbf{S}\,\mathbf{X} ,$$

where

$\mathbf{T} = (T_1,\ T_2,\ T_3 + L/N)$ as fractions of cell edge and

$\mathbf{S}$ = a counterclockwise rotation of $L{\cdot}M/N$ cycles about c* axis.

For example, the Pauling and Corey right-handed alpha helix repeats after 5 turns and 18 residues and can be represented by 18 symmetry cards with $N = 18$; $M = 5$; $L = 0, 1, \ldots, 17$; $T_1, T_2, T_3 = 0$. The input atom list contains the contents of one residue.

3.2.4 Atom Parameter Cards (1 $\leq$ NATOM $\leq$ 166). – Two cards are required for each input atom. The first contains the chemical symbol and positional parameters, and the second contains temperature factor

[3]Only symmetry cards for *general* symmetry equivalent positions are permitted. Symmetry cards which explicitly designate special positions such as *X, X, X; X, X, Z; X,Y,*0; ¼,*Y*,0; and ¼,¾,0 *are not allowed.*

information or other information which specifies how the atom is to be represented on the drawing. The format allows the use of the atom parameter cards produced by the FORTRAN Least Squares Program OR FLS by Busing, Martin, and Levy (1962).[4] Several alternate inputs are possible for each of the two cards, and the number in columns 55–63 denotes the type used on that particular card.

3.2.4.1 Positional Parameter Card. – FORMAT(A6,3X,5F9.6,F9.0)

Columns				
1–6	Up to six alphanumeric characters centered in the six-place field			
7–9	Blank			
	Type 0	Type 1	Type 2	Type 3
10–18	–	–	–	x_0 (A) Cartesian
19–27	–	–	–	y_0 (A) Cartesian
28–36	x (fractional, crystal)	x (A, crystal)	x (A, Cartesian)	r (A) cylindrical
37–45	y (fractional, crystal)	y (A, crystal)	y (A, Cartesian)	ϕ (°) cylindrical
46–54	z (fractional, crystal)	z (A, crystal)	z (A, Cartesian)	z (A) cylindrical
55–63	0 or blank	1	2	3

Type 0 is the normal input based on triclinic coordinates. Some authors give coordinates in A along the unit cell vector; type 1 would be used in such a case. Type 2 allows one to place a model described in Cartesian coordinates onto a general triclinic lattice. The orientation of the Cartesian system $x\ y\ z$ in the general lattice **a b c** is the standard type described in 3.1.8 with x along **a** and z along **c***. Type 3 is similar to type 2 except that cylindrical coordinates r, ϕ, z are used and the axis of the system can be displaced from zero in the $x\ y$ Cartesian plane by the displacement x_0, y_0. Cylindrical coordinates are often used in the literature to describe a helical structure. The x_0, y_0 translation should be zero if helical symmetry operators are used. This translation feature is meant to be used in explicitly describing the contents of a multiple helix cell.

3.2.4.2 Temperature Factor Card. – FORMAT(I1,F8.6,5F9.6,F9.0)

Columns						
1	A sentinel $\neq 0$ for last atom only					
	Type 0,1,2,3,10	Type 4,5,8,9	Type 6		Type 7	
2–9	b_{11}	U_{11}	B	B	R	R
10–18	b_{22}	U_{22}	0	0	0	0
19–27	b_{33}	U_{33}	0	[VDC$_1$]	0	[VDC$_1$]
28–36	b_{12}	U_{12}	0		0	
37–45	b_{13}	U_{13}	0	[VDC$_2$]	0	[VDC$_2$]
46–54	b_{23}	U_{23}	0		0	
55–63	0,1,2,3,10	4,5,8,9	6 (or 0)	6 (or 0)	7	7

[4]W. R. Busing and H. A. Levy, *A Fortran Crystallographic Least-Squares Program*, ORNL-TM-305 (Nov. 21, 1962).

The coefficients $b_{ij}(i,j = 1,2,3)$ of the anisotropic temperature factor, types 0,1,2,3,10, are defined as follows: The complete temperature factor is

$$(\text{Base})^{\{-D(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + c\, b_{12}hk + c\, b_{13}hl + c\, b_{23}kl)\}}$$

where in type 0: Base = e, $C = 2$, $D = 1$;

type 1: Base = e, $C = 1$, $D = 1$;

type 2: Base = 2, $C = 2$; $D = 1$;

type 3: Base = 2, $C = 1$, $D = 1$;

type 10: Base = e, $C = 2$, $D = 2\pi^2$.

The coefficients $U_{ij}(i,j = 1,2,3)$ of the anisotropic temperature factor types 4 and 5 are defined as follows: The complete temperature factor is

$$\exp\left\{ -D\ (a_1^{*2}U_{11}h^2 + a_2^{*2}U_{22}k^2 + a_3^{*2}U_{33}l^2 + Ca_1^*a_2^*U_{12}hk + Ca_1^*a_3^*U_{13}hl + Ca_2^*a_3^*U_{23}kl)\right\} ,$$

where a_1^*, a_2^*, a_3^* are reciprocal cell dimensions and in types 4 and 8, $C = 2$; in types 5 and 9, $C = 1$; in types 4 and 5, $D = \frac{1}{4}$; in types 8 and 9, $D = 2\pi^2$. Type 6 allows the input of the Debye-Waller isotropic temperature factor B, which is used as follows:

$$\exp\,(-B \sin^2 \theta/\lambda^2) ,$$

where λ is the wavelength and θ is the Bragg angle. The parameter B is related to mean-square displacement $\overline{\mu^2}$ of the atom from its mean position by the relation

$$B = 8\pi^2\, \overline{\mu^2} .$$

When the isotropic temperature factor is used, the atom is represented as an isotropic ellipsoid (sphere) with equal principal axes of length μ. When the field in columns 19–27 is 0 or blank, the directions of the principal axes are along the standard Cartesian system axes (see 3.1.8). However, one can reorient these arbitary orthogonal vectors by using the two vector designator codes VDC_1 and VDC_2; then the three new principal-axis vectors will be VDC_1, $(VDC_1 \times VDC_2)$, and $VDC_1 \times (VDC_1 \times VDC_2)$. This is strictly an artistic feature of no physical significance.

Type 7 allows the input of arbitrary spheres of radius $\overline{\mu} = R$ in angstroms. The vector triplet orientation is specified as with type 6. An additional feature allows one to use a completely blank card (except perhaps column 1) for a temperature factor card. In this case the program assumes type 7 with an $R = 0.1$ A.

A type 10 temperature-factor input card may be used to load Cartesian temperature factors having components in the standard Cartesian system (3.1.8). This feature complements the type 3 Cartesian positional parameter input system (3.2.4.1) and is useful for plotting mean-square displacements caused by internal molecular motions as calculated from spectroscopic normal-coordinate analyses.[5,6]

3.3 Instruction Input

The instructions are the commands used in programming an illustration, and there is no required sequence for the instructions, except as indicated by the programming logic. Some instructions require

[5] C. K. Johnson, chap. 9 in *Thermal Neutron Diffraction*, ed by B. T. M. Willis, p. 149, Oxford University Press, London, 1970.

[6] R. R. Holmes and R. M. Deiters, *J. Chem. Phys.* **51**, 4043 (1969).

trailer cards, which may have three different formats. The program is informed what the format of the next card will be with the "look ahead" field, columns 1 to 3. The program action is also influenced by this information.

"Look ahead" (columns 1–3)	Next card will be –	Program action
0 or blank	Format No. 0, a new instruction	Execute present instruction; then read next card.
1	Format No. 1, continuation of present instruction	Read continuation card; then check "Look ahead."
2	Format No. 2, vector search code	Read (VSC) card; then check "Look ahead."
3	Format No. 3, alphanumeric info.	Read alphanumeric info. and execute instruction; then read next card.

3.3.1 Instruction Cards. – *3.3.1.1 The Format No. 0 Instruction Card.* – FORMAT(I3,I6,7F9.0)

Columns	
1–3	"Look ahead" (0,1,2,3)
4–9	Instruction number
10–18	1st parameter
19–27	2nd parameter
.	.
.	.
.	.
64–72	7th parameter

3.3.1.2 Format No. 1, Instruction Continuation Card. – FORMAT(I3,I6,7F9.0) A maximum of 19 continuation cards per instruction is permitted.

Columns	
1–3	"Look ahead" (0,1,2,3)
4–9	Blank
10–18	8th parameter, or 15th, . . . , or 134th
.	.
.	.
.	.
64–72	14th parameter, or 21st, . . . , or 140th

3.3.1.3 Format No. 2, Vector Search Code (VSC) Card. – FORMAT(I3,6X,5I3,8F6.0) A maximum of ten VSC cards is allowed. These cards can be entered with any instruction, but only certain instructions will use them. They must be entered with the particular instructions that require them; that is, they are not held over. Table 3.1 will be referred to as the individual instructions are explained.

Table 3.1. Vector search code cards

Columns	Search instructions 101 402 102 412	Inertial axes 505/506	Bond plotting instructions 801/811/821	Bond plotting instructions 802/812/822	Bond plotting instructions 803/813	Negative No. in columns 43 to 48 802/812/822	Negative No. in columns 43 to 48 803/813
1–3	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead
4–9	–	–	–	–	–	–	–
10–12	ORG. ANR	ANR	–	ANR (A)	ANR (A)	ANR (A)	ANR (A)
13–15			–				
16–18	TAR. ANR	–	–	ANR (B)	ANR (B)	ANR (B)	ANR (B)
19–21		–	–				
22–24	–	–	Bond type	Bond type	–	Bond type	–
25–30	*D* min (A)	Weight	–	*D* min (A)	*D* min (A)	*D* min (A)	*D* min (A)
31–36	*D* max (A)	–	–	*D* max (A)	*D* max (A)	*D* max (A)	*D* max (A)
37–42	–	–	Bond radius (A)	Bond radius (A)	–	Bond radius (A)	–
43–48	–	–	Perspective label hgt. (in.)	Perspective label hgt. (in.)	–	ANR (P)	ANR (P)
49–54	–	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–		
55–60	–	–	Nonperspective label hgt. (in.)	Nonperspective label hgt. (in.)	–	D_p min (A)	D_p min (A)
61–66	–	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–	D_p max (A)	D_p max (A)
67–72	–	–	Digits indicator	Digits indicator	–	–	–

3.3.1.4 Format No. 3, Labeling Card. – FORMAT(12A6)

Columns

1–72 Up to 72 digits of alphanumeric label information centered about columns 36 and 37. Note: There is no "look ahead" column in Format No. 3; the next card must be a new instruction card. Instructions 902, 903, and 913 are the only ones which require this input. It may be used with other instructions as a device to transfer comments about the particular instruction to the monitor output listing.

3.3.2 Structure Analysis Instructions (100 Series). – This series of instructions is not connected with drawing illustrations. It is used to obtain on the standard output medium of the computer a convenient tabulation of the chemically interesting aspects of a crystal structure, such as interatomic distances, interatomic angles, and principal axes of thermal motion.

3.3.2.1 Instructions 101 and 102. – These instructions call subroutine SEARCH, which finds all "target" atoms within a sphere of enclosure of radius *D* max about a particular "origin" atom. The instruction card has an atom designator run (see 3.1.3) of origin atoms (Org. ADR) and an atom number run of target atoms (Tar. ANR). The Org. ADR allows one to calculate several spheres successively with a printout of results after each one. For example, suppose there are nine atoms in the input list and we want the total surroundings of atoms 365502, 465502, and 565502 out to a maximum radius, *D* max, of 4 A. The Org. ADR is designated (365502, 5) or (365502, 565502)[7] and the Tar. ANR is designated (1,9). Further selection of the interatomic vectors from a particular origin atom to the target atoms which fall within the limiting sphere is possible with vector search code (VSC) cards of Format No. 2 (see 3.3.1), which can be entered with the instruction. If VSC cards are present, then the vectors must also satisfy one of the VSC's in order to be saved. A VSC card to specify the selection of a shell of vectors in the above example might be coded as follows: Org. ADR (3,5) Tar. ANR (1,9) Dist. range (2.0, 2.7). More selective VSC's are also possible. They are meant to be based on known interatomic distance ranges, such as those tabulated in Vol. III of the *International Tables for X-Ray Crystallography.*[8]

Vectors found about a particular origin atom are stored in a table of dimension 200 sorted on distance. Duplicate vectors (not duplicate distances) are eliminated. If more than 200 acceptable atoms are found about an origin atom, the 200 shortest vectors are saved. At the end of the search about each origin atom, the distances are printed out along with the atom designator codes (ADC), chemical symbols, and triclinic crystal coordinates for the origin and target atoms. If the instruction is 102, all possible interatomic angles and interatomic distances for the edges opposite the angles are also calculated and printed for the stored vectors. There will be $n(n-1)/2$ angles for n vectors.

---

[7]For the origin sequence 355501, 455501, 555501, an Org. ADR input (3,5) is allowed as well as (355501,5) and (355501,555501); however, the Tar. ANR must always be designated as shown. In sect. 2.1, Org. ADR is designated as ORG 1, ORG 2; and Tar. ANR is denoted by TAR 1, TAR 2. A minus sign preceeding the second member of the Org. ADR is not required.

[8]H. Ondik and D. Smith, "Interatomic Distances in Inorganic Compounds," p. 257 in *International Tables for X-Ray Crystallography*, vol. III, ed. by K. Lonsdale, Kynoch, Birmingham, 1962.

The tabulation of atom designator codes, which is obtained automatically when these instructions are given, is often useful for planning an illustration. Although the tabulation is complete within the addressable region of 9^3 cells, the computing time is generally only a matter of seconds per sphere unless a very large *D* max is specified. Subroutine SEARCH is a rather elaborate routine designed to minimize computing time. This subroutine is also used for instructions 402 and 403, which are explained in 3.3.5.

Instruction card for instructions 101 and 102:

Columns	
1–3	0 or 2 (look ahead)
4–9	101 or 102
10–18, 19–27	Origin-ADR (atom designator run)
28–36, 37–45	Target ANR (atom number run)
46–54	D max (A)

3.3.2.2 Instruction 103. – Principal axes of thermal motion (or arbitrary spheres, according to the temperature factor input) for all atoms in the input list are calculated. The printout contains root-mean-square amplitudes of displacement along the principal axes of the trivariate normal probability density function and direction cosines for the principal axes relative to the reference Cartesian base vectors. A symmetric covariance dispersion matrix based on the reference Cartesian system is also printed out. The diagonal elements are the mean-square displacements along the reference Cartesian axes.

Columns	
1–3	0 or blank (look ahead)
3–9	103
10–18	Blank

3.3.2.3 Instructions 105 and 106, Convoluting Sphere of Enclosure and Reiterative Convoluting Sphere of Enclosure. – These instructions utilize the ATOMS table and can only be used after one or more atoms have been placed in the table by a 401, 402, 403, or 404 instruction. The contents of the table are returned to the condition of entry at the conclusion of instructions 105 and 106.

All atoms in the ATOMS table which have atom numbers within the origin atom number run (Org. ANR) of the instruction are used as origin points. Interatomic distances for all neighboring atoms (whether or not in the ATOMS table) are found out to the specified radius. Vector-search-code (VSC) cards may be used for screening if desired.

Instructions 105 and 106 are similar, except that instruction 106 keeps repeating the "convolution" process until no new atoms with atom numbers within the Org. ANR are found.

Instruction 106 is useful for molecular structures where the atoms in the input asymmetric unit do not form an intact molecule. In a case of this nature, it is advisable to place a single atom into the ATOMS table with a 401 instruction and let a 106 instruction find the molecule. Care must be taken to specify a D max which will enclose only bonded atoms. The 106 instruction should *not* be used for structures forming infinite chains.

Columns	
1–3	0 or 2 (look ahead)
4–9	105 or 106
10–18, 19–27	Origin ANR (atom number run)
28–36, 37–45	Target ANR (atom number run)
46–54	D max (A)

3.3.3 Plotter Control Instructions (200 Series). – The 200 series is a group of instructions that control the plotter initialization, frame advance, termination, and any other peripheral commands that are required for a particular equipment configuration or plotting package. When the program is modified for a different equipment configuration, these series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements. Instructions for controlling the CalComp 765 and 835 off-line magnetic tape plotting systems[9] are given here.

3.3.3.1 Instruction 201, Plot Package Initialization, Mechanical Plotter. – This instruction (or a 203 instruction) must be executed before any plotting can take place. It is a safe policy always to make this the first instruction card. It should be used only once per computer job regardless of how many plots are to be drawn during the job. If the 201 (203) and 301 instructions are omitted, all calculations are carried out but no plotting is done.

3.3.3.2 Instruction 202, Plot Terminate and Frame Advance. – This takes care of putting the correct plot termination information onto the magnetic tape to inform the plotter that the current plot is finished. It also allows advance of the paper so that the old plot is removed and new paper is in position for the next plot.

Columns	Instruction 201	Instruction 202
1–3	Blank	Blank
4–9	201	202
10–18	–	Plotter movement along *x* edge of paper in inches

[9]The CalComp is an incremental plotter. The particular Benson-Lehner model available at Oak Ridge Central Data Processing Facility has also been used. The Benson-Lehner is an electromechanical *x-y* plotter with an analog converter. In general it seems that an incremental plotter is better suited to the requirement of OR TEP. The user should be warned that in the author's experience the magnetic tape plotting systems are notoriously troublesome; an annoying percentage of plot failures is to be expected because of equipment malfunctions. (This was true in 1965 and is still true in 1975.)

3.3.3.3 Control Instructions for CalComp Model 835 Cathode-Ray-Tube Plotter. – In order to plot interchangeably on the CRT and the mechanical CalComp plotters, an extended 200 series of instructions is necessary.

A 203 instruction initializes the CRT plotter and is used in place of the 201 instruction. In general, no other changes are needed except that the plotting area specified by the 301 instruction must not exceed 17 in. in *x* and 11 in. in *y*. (The 301 primer constants are set accordingly.)

Columns		
1–3	Blank	
4–9	203	
10–18	XORG	(new position of the origin of plotter coordinates relative to the lower left-hand corner of the normal CRT plotting area)
19–27	YORG	
28–36	IZORG	(beam intensity origin)

The entries for XORG, YORG, and IZORG are normally zero or blank.

The beam intensity, IZ, can be changed from its initialized value IZ = IZORG + 18 to any other value in the range 0 to 30 with a 204 instruction. The usable range of IZ is about 12 to 24 with the higher values producing darker lines.

Columns	
1–3	Blank
4–9	204
10–18	IZ – IZORG

The frame advance instruction 202 is interpreted differently for CRT usage; however, the same 202 instruction cards used for a mechanical plotter plot can also be used for a CRT plot. Any positive number in columns 10 to 18 of the 202 instruction (3.3.3.2) will add a block address (i.e., plot number) to the magnetic tape and will advance the film to a new frame. A value of zero in columns 10 to 18 will add a block address but will not advance the film to a new frame, and a negative value will terminate the output magnetic tape file. It is not normally necessary to use the negative value option since the termination is taken care of automatically when the -1 instruction is executed if a 201 instruction was not executed after the 203 initialization instruction; however, if the mechanical plotter is to be used during the same job, the negative value option allows the CRT to be terminated properly before initialization of the mechanical plotter.

3.3.4 Plot Boundary Instructions (300 Series). – This is a set of miscellaneous instructions for specifying the dimensions of the drawing, viewing distance, general lettering orientation, and pen displacement for line retracing.

3.3.4.1 Instruction 301. – This instruction defines the limiting *x* and *y* dimensions, in inches, of the plot boundary and the border indentations. The boundary dimensions must not exceed those allowed by the plotter. The program will prevent the pen from getting closer than 0.1 in. to any boundary. The border indentation is an equal margin inside the entire boundary. When automatic scaling is used (600 series), the center points of the atoms are prevented from falling in the margin; but the atom represen-

tation, which has a finite size, may extend into that area. To compensate for the overlap, the border dimensions should be large when the overall drawing scale and the ellipsoid scale are expected to be large.

In addition, instruction 301 specifies the perspective viewing distance, in inches, from the plane of the drawing. An entry of 0 for view distance is used to indicate an infinite view distance, and the crystal structure is then mapped in parallel projection normal to the drawing board.

Columns		Primer Constant
1–3	–	–
4–9	301	–
10–18	Plot *x* limit (in inches)	17.
19–27	Plot *y* limit (in inches)	11.
28–36	View distance (in inches)	0. (parallel proj.)
37–45	Border (in inches)	0.5

3.3.4.2 Instruction 302, Title Rotation. – For regular titles and chemical symbols, the title rotation is specified with instruction 302. The lettering base line for all lettering is rotated counterclockwise by an angle theta, in degrees, from the *x* axis of the plotter. Although any value is allowed, 0° and –90° are the values most often used, so that, when one views the finished drawing, either the *y* plotter axis is vertical or the *x* plotter axis is vertical.

Columns		Primer Constant
1–3	Blank	–
4–9	302	–
10–18	Theta in degrees	0.

3.3.4.3 Instruction 303, Retrace Displacement. – For artistic purposes, certain lines are made heavier than others by retracing over the path several times with slight pen displacements (DISP) from the original path. For example, in drawing ellipsoids the forward half of the principal plane trace is made heavier than the hidden half so the eye does not confuse the two halves. In addition all regular lettering (but not perspective lettering) is gone over four times to give it boldface appearance. In preliminary runs or when the plotter is not of the incremental type, this embellishment may be objectionable to the user because of the increased computing and plotting times (particularly the latter). All retracing can be eliminated by setting DISP = 0. The primer parameter for DISP is 0.005 in., which is the resolution of the CalComp plotters at ORNL. For other plotters or for various inking pen sizes, DISP can be reset at the user's discretion. Retracing should not be used with a CRT plotting device.

Columns		Primer Constant
1–3	–	–
4–9	303	–
10–18	DISP (in inches)	0.005

3.3.5 Atom List Instructions (400 Series). – This series allows the user to specify which atoms are to be included in the illustration. The atom designators for the chosen atoms are stored in the ATOMS array for future use by other instructions. The ATOMS array can hold 500 atoms; but if the intended illustration has more than this, the illustration can be segmented and the segments drawn sequentially on the same plot.

Groups of atoms are added to or eliminated from the ATOMS array (which is set to zero at the start of the program) with the 400 and 410 series respectively. The groups can be denoted by atom designator runs (see 3.1.3), spheres of atoms about any center point (see 3.1.6), and boxes of atoms centered on any point (see 3.1.7). Duplicate entries of the same atomic position are prevented by the program. The content of the ATOMS list is printed on the monitor output tape after each 400 series instruction.

3.3.5.1 Instructions 401 and 411, Atom Designator Run Add and Atom Designator Run Eliminate. – These instructions can contain: (*a*) atom designator codes (ADC) for a single atom, (*b*) atom designator runs (ADR) for several atoms in a run, (*c*) blank fields (except between the two entries of a run), and (*d*) any combinations of (*a*), (*b*), and (*c*). Since up to 19 Format No. 1 continuations are possible per instruction, up to 70 runs can be made per instruction and an unlimited number of instructions can be used. The ATOMS list, however, will only accept the first 500 atoms.

Columns	
1–3	Blank or 1 (depending on what follows)
4–9	401 or 411
10–18	As described above
.	
.	
.	
64–72	

3.3.5.2 Instructions 402 and 412, Sphere of Enclosure Add and Sphere of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete, partial, or vector screened, see 3.1.6) of a sphere of enclosure about any addressable point. For instruction 402, the contents of the spheres are *added to* the atom list except for positional duplications, which are omitted. In the 412 instructions, all points in the spheres are *eliminated from* the atoms list if they are present in that list. The instructions call subroutine SEARCH, and the instruction input details are identical to those of instructions 101 and 102 (see 3.3.2.1) except for the instruction number. In the monitor output, only the ATOMS list atom designator codes are printed and not the coordinates and interatomic distances. If the origin atoms on which the spheres of enclosure are centered are to be saved, the target atom number run (Tar. ANR) must contain this atom number. Furthermore, if vector search code cards of Format No. 2 are used, one of them must satisfy the intra-atom null vector for the origin atom in order to retain it.

3.3.5.3 Instructions 403 and 413, Box of Enclosure Add and Box of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete or partial but *not* vector screened, see 3.1.7) of a box of enclosure about any addressable point (or atom designator run of addressable points). The three axes of the box are parallel to the three base vectors of the reference Cartesian system, and the *semidimensions* of the box are specified on the instruction card. If an orientation of the box different from the standard orientation (see 3.1.8) is desired, than a 501 or a 502 instruction, or both, should be used before this instruction to reorient the reference Cartesian system. After this instruction has been executed, the reference system can undergo further reorientation as desired for plotting purposes, etc.

As in the case of the sphere of enclosure (see 3.3.5.2), the origin atom on which the box is centered will not be included unless the target atom number run includes the origin atom number. Vector search codes are not used by this instruction. Subroutine SEARCH is used by this instruction, and the instruction input details are similar to those described in 3.3.2.1 except that D max is replaced by the semidimension $a/2$ of the box and the following fields on the card are used to specify the other two semidimensions $b/2$ and $c/2$. One must use caution in choosing the box dimensions so that the atom table does not overflow.

Columns	
1–3	Blank
6–9	403 (or 413)
10–18	Origin ADR (see 3.3.2.1)
19–27	
28–36	Target ANR (see 3.3.2.1)
37–45	
46–54	$a/2$ (A)
55–63	$b/2$ (A)
64–72	$c/2$ (A)

3.3.5.4 Instructions 404 and 414, Triclinic Box of Enclosure Add and Triclinic Box of Enclosure Eliminate. – These instructions are similar to instructions 403 and 413, except that the triclinic box of enclosure is bounded by planes parallel to the principal planes of the crystal lattice. The semidimensions $a/2$, $b/2$, $c/2$ refer to fractional (triclinic) coordinates. To specify the contents of the conventional unit cell, one would use $a/2 = b/2 = c/2 = .5$, and the Org. ADR would refer to a point in the input atom list at 1/2, 1/2, 1/2.

3.3.5.5 Instructions 405, 406, 415, 416; Convoluting Sphere of Enclosure Add, Reiterative Convoluting Sphere of Enclosure Add, Convoluting Sphere of Enclosure Eliminate, and Reiterative Convoluting Sphere of Enclosure Eliminate. – These instructions are used in the same manner as instructions 105 and 106 (see 3.3.2.3). Their function is to add atoms to or eliminate atoms from the ATOMS table. A valid origin atom must be placed in the ATOMS list with a 401, 402, 403, or 404 instruction before the present instructions are used. All atoms in the ATOMS table which have atom numbers within the origin atom number run (Org. ANR) of the instruction are used as origin points of convolution.

An important use for the 405 instruction is to complete the coordination shells around metal atoms without having to describe any of the atoms individually. Another use might be to obtain a cluster of atoms out to the *n*th neighbor when only the distance to the first neighbor is known. This can be accomplished by using *n* consecutive 405 instructions with D max slightly more than the first neighbor distance.

Instruction 406 is useful for describing molecular compounds when an unfortunate choice of atoms for the input asymmetric unit does not allow the molecule to be described by a run. D max must be chosen judiciously so that the search does not cross molecular boundaries.

The input format is identical to that described in 3.3.2.3, with the appropriate instruction number in columns 4–9.

3.3.5.6 Option for Examining E-Map Results. – Stereoscopic drawings are useful for the rapid screening of *E* maps when direct methods are used for solving crystal structures. First the interpolated positions of the largest peaks in the Fourier synthesis *E* map are punched on cards directly by a Fourier program. Then OR TEP starts at a given peak (usually the largest) and does a reiterative-sphere-of-enclosure-add instruction (406) to isolate a molecule if one is present. In order to terminate the convolution procedure when extraneous "bridging peaks" link the molecules, a modification was added to the 406 instruction which allows an atom (in any of its equivalent positions) to be entered in the ATOMS list only once. To invoke this feature, a type 1 continuation card (3.3.1.2) with a 1 in column 18 is added to the 406 instruction. The 406 instruction operates normally if the continuation card is omitted (3.3.5.5).

3.3.5.7 Instruction 410, Clear Atoms List. – This instruction clears the atoms list to zero. When the program is first entered, the list is automatically set to zero.

3.3.6 Orienting Instructions (500 Series). – This series of instructions orients the reference and working Cartesian systems (see 3.1.8). Each time the reference system is redefined with a 501 or rotated with a 502, the working system is automatically made coincident with the reference system. The working system can be displaced from the reference system by rotating about an axis of the reference system with a 503 instruction. The working system is always positioned by a rotation from the reference system and does not depend on the previous working system orientation. After each 500 series instruction, the base vectors of the relevant Cartesian system are printed out. These vectors are based on the triclinic coordinate system. The postfactor transformation matrix for converting from triclinic coordinates to Cartesian coordinates is also printed out. The inverse transformation matrix may be formed by placing the three base vectors together in row vector form.

3.3.6.1 Instruction 501, Reference Cartesian System Assignment. – Any Cartesian coordinate system is based on three orthonormal base vectors and an origin point. The origin point in the model (ORGN) is specified with an atom designator code. The three orthonormal base vectors can be described by two noncollinear vectors, and OR TEP provides the two following separate techniques for performing this operation, using vector cross products of the two vectors **u** and **v**.

	Type A	Type B
Base vector 1 (x axis)	$\mathbf{u}$	$\mathbf{u}$
Base vector 2 (y axis)	$\mathbf{u} \times \mathbf{v}$	$(\mathbf{u} \times \mathbf{v}) \times \mathbf{u}$
Base vector 3 (z axis)	$\mathbf{u} \times (\mathbf{u} \times \mathbf{v})$	$\mathbf{u} \times \mathbf{v}$

The reference system x and y axes will parallel the plotter x and y axes, and the origin point ORGN will lie in the plane of the plotter. The viewer will be looking into the z axis vector of the coordinate system from a distance VIEW in inches (see 3.3.4.1) directly above the origin point.

Columns		Effective Primer Constant
1–3	–	–
6–9	501	–
10–18	Origin (ADC)	000000
19–27	Vector $\mathbf{u}$ (VDC)	155501
28–36		165501
37–45	Vector $\mathbf{v}$ (VDC)	155501
46–54		156501
55–63	–	–
64–72	0 = Type A, >0 = Type B	1

3.3.6.2 Instruction 502, Reference Cartesian System Rotation. – The crystal model can be given any orientation desired with a series of rotations of the model about the reference system axes. In general, three rotations (e.g., those of an Eulerian system) are sufficient to achieve any orientation, but for convenience an unlimited number of rotations are permitted in the program. In addition, rotations of 120° about the body diagonal of the reference Cartesian system are permitted (this is achieved by a cyclic permutation of reference base vectors).

Each operation requires two fields in the instruction card. For axial rotations, the first field of each pair will have the number 1, 2, or 3 to indicate rotation about the x, y, or z axes of the reference system. The second field will have the rotation angle in degrees for a right-handed rotation of the model about the designated axis (i.e., a positive angle signifies a counterclockwise rotation of the structure with the designated axis pointing toward the reader). The body diagonal rotation is designated by either a (– 1) or a (– 2) in the first field to indicate a 120° or a 240° right-handed rotation about the body diagonal, and the second field is blank. A (– 3) would rotate the structure completely around and thus not change its previous orientation.

Columns	
	First Card
1–3	0 (or 1 if continued on next card)
4–9	502
10–18	1,2,3,−1,−2
19–27	ϕ_1°
28–36	1,2,3,−1,−2
37–45	ϕ_2°
46–54	1,2,3,−1,−2
55–63	ϕ_3°
64–72	1,2,3,−1,−2
	Second Card
10–18	ϕ_4°
.	
.	
.	

If desired, each rotation can be executed with a separate 502 instruction card.

3.3.6.3 Instruction 503, Working Cartesian System Rotation (Stereoscopic Rotation). – The working (minor) Cartesian system is automatically made coincident with the reference system whenever the reference system is redefined with a 501 instruction or rotated with a 502 instruction. To define an orientation of the working system which is not coincident with the reference system we use a 503 instruction, which allows one rotation about one axis of the reference system. Actually any number of successive rotations can be made, but the effect is not cumulative since the starting point for each rotation is always the reference system. Body diagonal rotations are not permitted.

A 503 rotation normally precedes each member of a stereoscopic pair of plots. The rotation is about axis 2 if the stereo pair is to be viewed with the x axis parallel to the observer's interocular line and about axis 1 if the y axis is to be parallel to that line.

Columns	
1–3	–
4–9	503
10–18	1,2,3
19–27	ω°

3.3.6.4 Optimal Parameters for Stereoscopic Drawings. – Figure 3.1 shows a geometrical construction which may be used to derive the parameters used in making stereoscopic drawings.[10,11] The empirical parameters in common usage [(*a*) 30-in. view distance, (*b*) 5° to 6° stereo rotation, and

[10] J. T. Rule, *J. Opt. Soc. Am.* **28**, 313 (1938).

[11] B. G. Saunders, *Appl. Opt.* **7**, 1499 (1968).

(c) a photographic reduction to achieve 2.2 to 2.4 in. separation of equivalent points] produce quite satisfactory results with a slightly exaggerated impression of depth. Theoretically, the best stereoscopic fidelity is obtained by translation of the origin rather than by stereo rotation of the object;[11] however, the comparison of results given in Fig. 3.2 shows that the differences are indeed minor and nearly impossible to detect. Stereo by translation of origin is achieved with instruction 504, which may be used in place of the 503 instruction; however, the 504 instructions should not be used when the ellipsoids have internal structure because the octants selected for shading may not be the same on both stereo views.

Columns

1–3	Blank
4–9	504
10–18	Translation of origin along x axis of reference system (in.)
19–27	Translation of origin along y axis of reference system (in.)
28–36	Translation of origin along z axis of reference system (in.)

For the geometrical conditions depicted in Fig. 3.1, the stereo-rotation instructions for the left and right eyes,

503 2 2.45

and

503 2 –2.45 ,

are replaced by the stereo translation instructions

504 –1.28 0 0

and

504 2.56 0 0 ,

respectively. If additional drawings are to be made, the origin first should be returned to its original position with the instruction

504 –1.28 0 0 ,

in order to prevent confusion.

3.3.6.5 Instruction 505, Origin at Centroid. – This instruction finds the first moment (i.e., centroid or center of gravity) of the atoms in the ATOMS list and makes this point the ORIGIN of the reference and working coordinate systems. A weighting scheme and screening may be applied to the atoms by using format No. 2 trailer cards (see Table 3.1). If no trailer cards are used, all atom positions are entered with unit weights.

3.3.6.6 Instruction 506, Origin at Centroid and Inertial Axis Coordinate System. – The calculation described for instruction 505 is performed; then the second moment matrix about the centroid is calculated, and the reference and working coordinate systems are set up along the principal axes of this matrix. This principal axis system of coordinates is along the inertial axis of the configuration of atoms in the ATOMS list. The x axis is along the long axis of the configuration (i.e., the minimum axis of inertia) and the z axis is along the short axis of the configuration (i.e. the maximal axis of inertia). The overlap

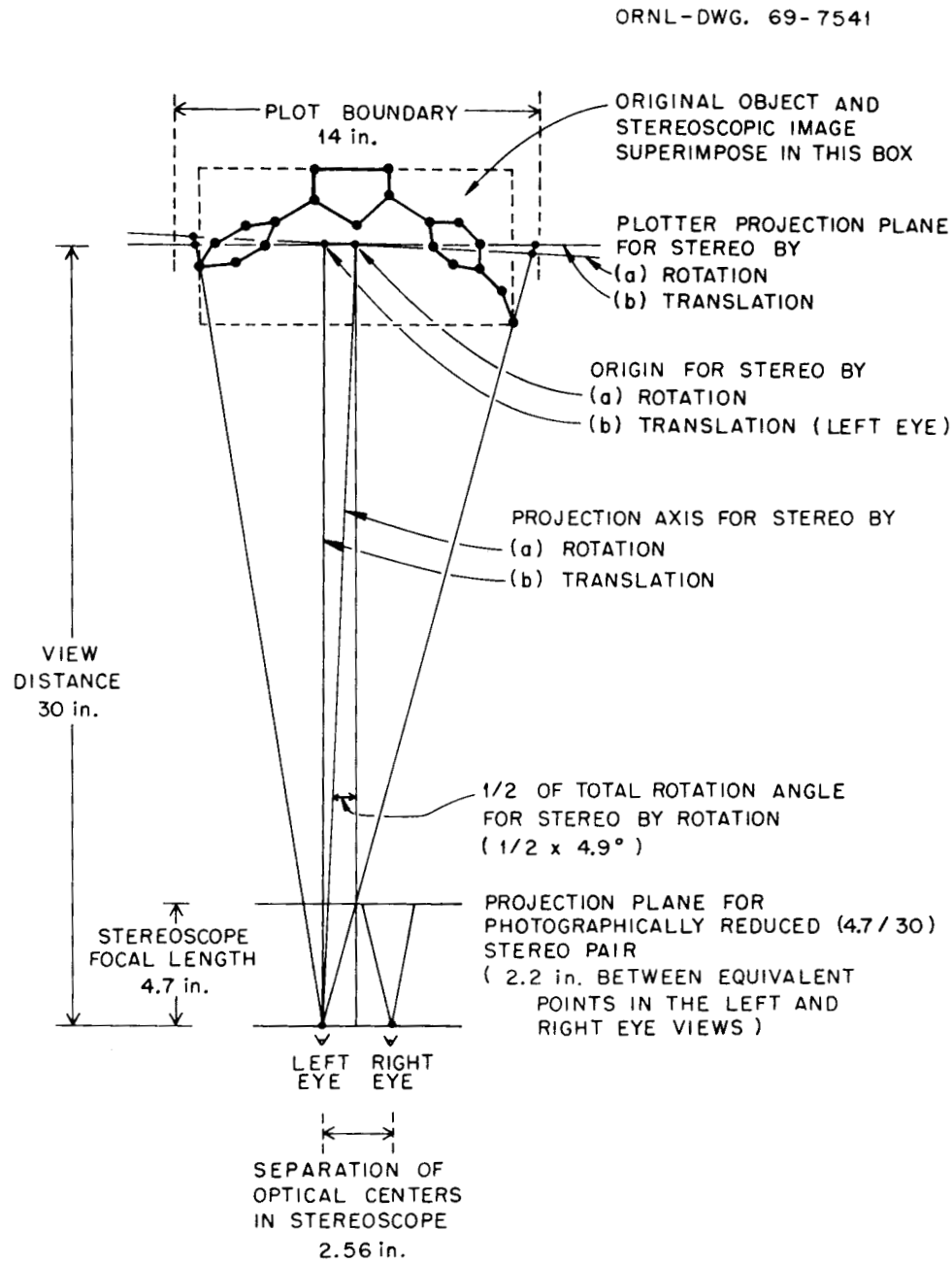

Fig. 3.1. Geometrical Relations Among the Stereoscopic Perspective Projection Parameters for a Typical OR TEP Drawing. The available plotting area for each projection is assumed to be 14 in. horizontally and at least 11 in. vertically. The scaled mathematical object is within a box 12 in. wide, 9 in. (or more) high, and 6 in. deep with the plane of the plotter halfway back into the box. The stereoscopic image seen through a stereoscope with a 12-cm (4.7-in.) focal length and a 6.5-cm (2.56-in.) separation between optical centers should appear superimposed on the original object. The parameters for both "translation stereo" and "rotation stereo" are shown. The appropriate linear dimensions can be scaled to accommodate other plotting areas and still produce the same final image.

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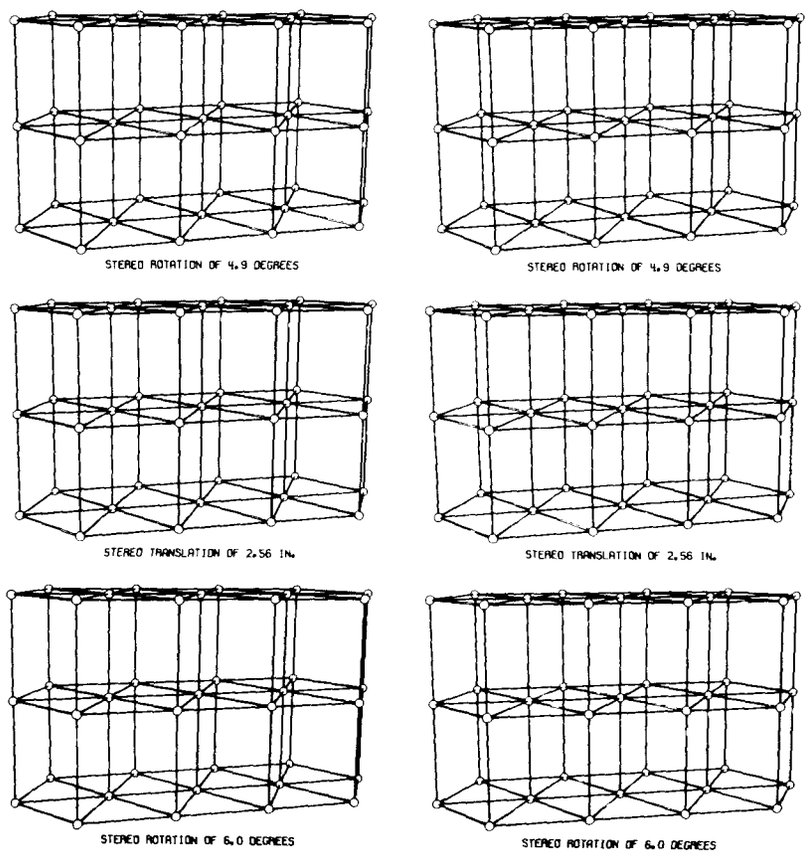

Fig. 3.2. Three Stereoscopic Drawings of a Hexagonal Lattice with Different Stereoscopic Parameters. The top and middle drawings utilize the parameters derived in Fig. 3.1 and demonstrate that the differences predicted (ref. 11) for translation and rotation stereo are not discernible in practice. The bottom stereo drawing illustrates the slight exaggeration in depth which occurs when a larger stereo rotation angle is used. The drawings should be viewed individually with a 12-cm focal-length stereoscope of good optical quality.

along the z-view direction is often minimized by this option. Furthermore, the x-y plane is the least-squares best plane for the atomic configuration. Format No. 2 trailer cards may be used to supply weights and screening (see Table 3.1).

3.3.6.7 Instruction 511, Overlap Elimination. – See Section 3.3.14.

3.3.7 Positioning and Scaling Instructions (600 Series). – These instructions are used to direct the placement of the origin point ORGN (specified by instruction 501) onto the drawing (dimensioned by instruction 301). In addition the three-dimensional assembly of atoms (chosen by the 400 series instruction) constituting the model is scaled. The atomic centers of the model will then be hanging in space above and below the drawing board correctly positioned to be projected from the eye point described with 301.

3.3.7.1 Normal Modes of Positioning and Scaling. – Several normal modes of operation are available to the user for positioning and scaling the model. Instruction 601 requires the user to supply a complete explicit description of position (x_0, y_0) and scale (SCAL1). At the other extreme, instruction 604 automatically scales and positions the model so that the peripheral projected atom centers will touch two

opposite borders and the peripheral atoms in the remaining dimensions will be centered on the drawing. An intermediate mode is available through 602, which provides automatic scaling after explicit positioning. In general this allows only one edge of the model to touch a border. Finally, instruction 603 requires an explicit scale and does automatic centering.

In general the 604 instruction is the easiest and safest one to use, but situations arise in which the user should not relinquish control to the program. For example, if a big illustration is to be drawn piecewise on a small plotter, the user will have to maintain control over the scale, and probably over positioning, so that the partial plots can be fitted together correctly.

A second scale factor SCAL2 is required in connection with the ellipsoid (or sphere) size. It is a dimensionless scale factor ratio used to modify all rms displacement values before plotting equiprobability ellipsoids or spheres. A table of SCAL2 values vs probability is given in Sect. 5.2. The primer constant for SCAL2 is 1.54, corresponding to 50% probability. If the instruction's entry for SCAL2 is 0 or blank, then SCAL2 is not modified by the instruction. The same statement also holds for x_0, y_0, and SCAL1. That is, if the instruction entry is zero or blank for any of these, then the value of the constant in memory is not changed. This means that an x_0 or y_0 cannot be entered as exactly zero, so that if zero is wanted, a small nonzero number should be entered.

Columns	601	602	603	604	Primer Constant
1–3	–	–	–	–	–
4–9	601	602	603	604	–
10–18	x_0	x_0	–	–	8.5
19–27	y_0	y_0	–	–	5.5
28–36	SCAL1	–	SCAL1	–	1.0
37–45	SCAL2	SCAL2	SCAL2	SCAL2	1.54

3.3.7.2 Incremental Modes of Positioning and Scaling. – Additional flexibility is provided through the incremental instructions 611, 612, and 613. These allow the user to "nudge" the model or modify the scale factor (SCAL1), or both, after the parameters have been initially set with a previous 600 series instruction. The 611 instruction adds Δx_0, Δy_0 to the previous x_0, y_0 position for the ORGN placement and multiplies the existing SCAL1 by ΔK (except if $\Delta K = 0$, SCAL1 is unmodified). Instruction 612 increments the position and then does an automatic scaling; 613 first increments the scale (by multiplying by ΔK) and then automatically repositions.

A conservative general approach is to follow a 604 with a 611 having $\Delta x_0 = 0$, $\Delta y_0 = 0$ and $\Delta K = 0.9$. This will simply reduce the scale 10% so that there is more space for labels, etc.

Column	611	612	613
1–3	–	–	–
4–9	611	612	613
10–18	Δx_0	Δx_0	–
19–27	Δy_0	Δy_0	–
28–36	ΔK	–	ΔK
37–45	SCAL2	SCAL2	SCAL2

3.3.8 Atom Plotting Instructions (700 Series). – These instructions are concerned with drawing various representations of the atom based on the familiar ball-and-stick molecular model. The ball in the general case is an ellipsoid representing a contour surface of equal probability density. Alternatively, when thermal motion is not being portrayed, the ball can be a sphere of arbitrary dimension. The 700 series also has provision for labeling the atomic site with the corresponding chemical symbol. The instructions in this series draw the "ATOMS list" atoms which project onto the usable part of the drawing area. Atoms found to be out of bounds are bypassed, and a Fault Message (NG = 10) is printed on the monitor output. An atom is out of bounds under the following conditions: (1) if its z coordinate in the scaled reference Cartesian system is greater than $\frac{1}{2}$ the viewing distance, (2) if its center after projection falls outside the limiting boundary of the drawing board, or (3) if the projected center is within $\frac{3}{4}$ of the margin width (BRDR) of a limiting boundary.

An ellipsoid, for graphical purposes in OR TEP, is considered to be composed of ellipses and straight lines. The ellipses are of two types, principal ellipses and boundary ellipses. Relative to the viewpoint, a principal ellipse is further subdivided into a front half and a back, or hidden, half. There are three principal ellipses per ellipsoid, corresponding to the three principal planes. The boundary ellipse is the edge of the ellipsoid as seen from the viewpont. The front and back halves of the principal ellipses meet at the boundary ellipse. The straight-line segments of the OR TEP ellipsoid are the forward principal axes, reverse principal axes, and octant shading lines.

Figure 3.3 shows various combinations of these elements. It is obvious that certain of these combinations are better representations than others. Instruction 701 generates the 5A model of Fig. 3.3, instruction 702 generates 2A, and 703 produces 3B. Instruction 704 draws the boundary ellipse alone. If an atom is entered as a sphere, the boundary will be circular before projection and slightly elliptical after perspective projection. Instruction 705 allows the user to make up any representation from the basic components.

Chemical symbols up to six alphanumeric characters in length are included with the input structural parameters for each atom. These symbols can be put onto the illustration with one 700 series or several 900 series instructions. The 700 series places the center of the six-character field of each atom in the same position relative to the atom center; the 900 series allows the user to position each symbol individually. The 700 series requires only three parameters as follows: (1) symbol height in inches, (2) parallel (left-right) offset in inches, and (3) perpendicular (up-down) offset in inches. The parameters refer to the model before projection, and they will change slightly during perspective projection. The parallel and

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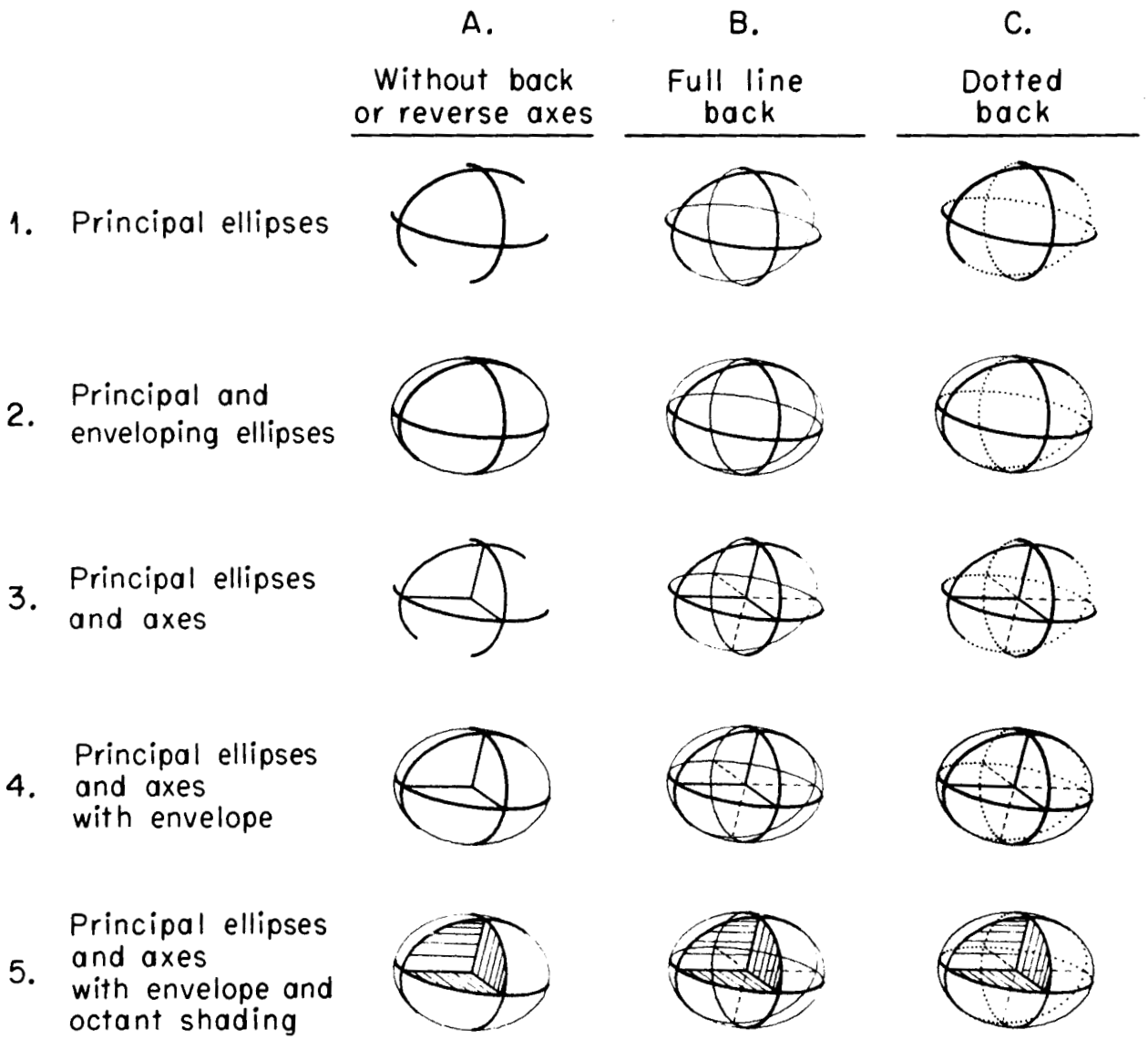

Fig. 3.3. Various Combinations of Ellipsoid Components.

perpendicular offset refer to the exact center of the six-character input field and are relative to the lettering base line set up with the 302 theta rotation. A symbol height of 0 or blank will cause the symbol-drawing routine to be bypassed.

In order to distinguish certain atoms, such as those in disordered positions, a 705/715 instruction with NPLANE = 4, NDOT = 3, 4, 5, or 6, NLINE = 0, and NDASH = 0 may be used to produce dotted boundary ellipses to contrast with the normal solid line boundary ellipses. Another feature of the 705/715 instruction is that if NPLANE = 0, and if the symbol height is greater than zero, then chemical symbols alone are drawn on the atomic sites.

It is possible to vary the thickness of the boundary ellipse line by making it a function of z, the height of the atom from the drawing board. This option is normally used with the 704 (boundary only) instruction but will work for any 700 instruction. Entries are put in the A_0 and A_1 fields of the instruction continuation card to specify the coefficients of

$$\Delta R(z) = A_0 + A_1 z ,$$

where

ΔR is the increase in radial dimension to be added to the width of the single pen line,

A_0 is ΔR for an atom at $z = 0$, and

A_1 is the rate of increase in radial dimension with z.

As an example, assume that the atoms of the scaled model range from 5 in. below to 5 in. above the drawing board and the pen width is 0.2 mm (.008 in.). If we want the closest ellipse boundary to be five times as wide as the farthest, then $\Delta R(-5 \text{ in.}) = 0$, $\Delta R(5) = 0.008 \times (5 - 1) = 0.032$ in.; thus $A_0 = 0.016$ in. and $A_1 = 0.0032$ in.

The program widens the line by stepping radially in increments of DISP, which is set by primer constant to 0.005 in. A 303 instruction can be used to change DISP if desired.

Selected types of atoms from the ATOMS table can be drawn without having to alter the contents of the table. This is accomplished by using an atom-number-run (ANR) code which includes the atom types that are to be drawn with a particular 700-series instruction. This feature is particularly useful when two or more different representations are used such as for the carbon and hydrogen atoms in the cubane example. If no ANR is entered, then all atoms in the table are drawn.

The monitor output for the 701 through 705 instructions consists of the following:

1. x,y plotter coordinates: the coordinates, in inches, for the projected atom center on the plot, measured from the lower left-hand corner of the limiting boundary. This is the fixed plotter coordinate system with origin point set by the plotter operator.

2. x,y,z working Cartesian coordinates: the coordinates, in inches, for the oriented and scaled atomic model before projection. The x and y axes parallel the plotter x and y axes, and the origin of the system is in the plane of the plotter at the point x_0,y_0 (see 3.3.7) in plotter coordinates. The point ORGN of the scaled model is at this point (see 3.3.6.1).

3. x,y,z triclinic coordinates, in fractions of the unit-cell edges relative to the crystal unit-cell origin.

4. Principal axes of thermal motion, consisting of (*a*) principal values of root-mean-square displacement and (*b*) direction cosine for principal vectors relative to the working Cartesian system.

5. The atom designator code and chemical symbol for the atom.

Instructions 711 through 715 are identical to 701 through 705 except that *the 710 series suppresses all monitor output except fault messages.*

3.3.8.1 Atom Plotting Instructions 701, 702, 703, 704, and 711, 712, 713, 714. –

Columns	
	First Card
1–3	1 (if boundary retracing or atom selection is desired; otherwise 0)
4–9	701, 702, 703, 704, 711, 712, 713, 714
10–45	Blank
46–54	Symbol height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
	Second Card (needed only for boundary retracing or atom selection)
1–3	Blank
4–9	Blank
10–18	A_0 (in.) or blank
19–27	A_1 (in.) or blank
28–36, 37–45	ANR or blank

3.3.8.2 Atom Plotting Instructions 705 and 715. –

Columns	
	First Card
1–3	1 (if boundary retracing or atom selection is desired; otherwise 0)
4–9	705 or 715
10–18	NPLANE = 0, no ellipsoid components = 1, boundary ellipse only = 3, principal ellipses only = 4, boundary + principal ellipses
19–27	NDOT (back side of principal ellipses) <0, solid line back side = 0, back side omitted = 3, 4 dots on back side = 4, 8 dots on back side = 5, 16 dots on back side = 6, 32 dots on back side
28–36	NLINE (forward principal axes and shading) = 0, no forward axes or shading = 1, forward principal axes only = N, forward axes + $(N - 1)$ line shading
37–45	NDASH (dashed reverse principal axes) = 0, no reverse axes = N, dashed reverse axes with N dashes
46–54	Symbol height (in.)
55–63	Parallel offset (in.) } for symbols
64–72	Perpendicular offset (in.) } for symbols
	Second Card same as 701

3.3.9 Bond Plotting Instructions (800 Series). – The bond plotting instructions are grouped into two general types, explicit and implicit, depending on how the bonds are specified. Explicit bonds require a vector designator code (see 3.1.2) for each bond. Implicit bonds make use of vector search codes (see 3.1.5) to find pairs of atoms from the ATOMS array set up by the 400 series instructions.

There are two types of bonds that can be drawn, stick bonds and line bonds. The line bond is a very crude, but rapid, method useful in drawing preliminary illustrations. It is constructed by placing centered symbols (e.g., +, ×, *, etc.) on the two atom sites and drawing a single straight line between them. Line bonds are always specified implicitly (803, 813 instructions).

The more elaborate bond is the stick bond, which could also be called a conical bond because of its accentuated perspective taper.[12] Each end of the bond intersects either (1) an ellipsoid or (2) an enveloping cone (tangent cone) which has its apex at the viewpoint and is tangent to an ellipsoid. In general, the ellipsoid intersection is automatically used if the axis of the bond intersects the ellipsoid at a point which is visible to the viewpoint; otherwise, the tangent cone intersection is used, so that the bond appears to terminate at the boundary of the ellipsoid. However, the user can specify that the ellipsoid intersection always be used in order to make the skeleton type model (e.g., 3B of Fig. 3.1) appear even more transparent. The radius of the stick bond and the number of lines which are used to draw the bond are specified by input parameters.

Bond-distance labels can be drawn automatically with stick bonds, but not with line bonds. The bond-distance label numbers are in Angstrom units to one, two, or three places past the decimal point. The bond labels on the illustration will have their base lines parallel to the stick bonds and will be right side up for the viewer. The height of the label in inches and the perpendicular offset distance for the center of the label relative to the center of the bond are parameters to be specified by the user. With the present primer constant for FORE, if the sine of the angle between the bond and the mean viewing vector is greater than 0.5, the lettering is done in perspective along the bond. When the sine of the angle is less than 0.5, the perspective lettering would be excessively foreshortened; the lettering is then made parallel to the plane of the drawing with its base line parallel to the projected bond. Different lettering heights and different perpendicular offset distances can be assigned to the perspective and nonperspective bond-distance labels.

All bond parameters are input with Format No. 2 trailer cards (see 3.3.1). The bond parameters are as follows:

1. Bond type (for stick bond) is designated by an integer NBOND, where $-5 \leqq \text{NBOND} \leqq 5$. The negative integers denote that both ends of the bonds terminate at the ellipsoids. The positive integers denote bonds ending either at the ellipsoid or the tangent cone, as described previously in this section. An entry of zero draws no bond. A magnitude of 1 for NBOND produces two lines, one for each bond edge, 180° apart in the plane normal to the bond axis. Lines are drawn 90°, 45°, 22.5°, or 11.25° apart for NBOND magnitudes of 2, 3, 4, or 5, respectively. The back side of the bond is not drawn. Representative samples are shown in Fig. 6.1.

[12]The accentuated taper may be increased or decreased by changing the value assigned to TAPER in SUBROUTINE PRIME (see TAPER in sect. 4.5).

2. The bond radius (mean value for stick bonds) is in Angstrom units. Values between 0.01 and 0.06 A usually give good results. Any positive value may be used as long as it is smaller than the scaled ellipsoid minimum semidimension. The bond radius is not changed by the ellipsoid scale factor ratio SCAL2. The bond radius should not be made "vanishingly small" (e.g., $r < 0.005$ A) if the overlap feature is used because numerical rounding may cause incorrect hidden-line elimination.

3. The height of perspective labels for bond distances is entered as zero if no bond distances are to be labeled. Positive values denote the lettering height in inches before projection.

4. The perpendicular offset for bond distance perspective labels (in inches) pertains to offset of the center of the distance label relative to the center of the bond.

5. The height of regular labels for bond distances is entered as zero if no bond distances corresponding to foreshortened bonds are to be drawn. Positive values give the lettering height in inches before projection.

6. The perpendicular offset for bond-distance regular labels has the same definition as parameter 4 above.

7. The significant digits indicator is -1, 0, or 1, denoting bond distance labels with one, two, or three digits, respectively, after the decimal place.

The use of vector-search-code (VSC) cards for the bond plotting instructions 802 and 803 has been extended to include a provision for drawing coordination polyhedra while suppressing the unwanted bonds. In addition to describing the bond with ANR(A), ANR(B), and the D min to D max range, a condition can be imposed to require that both atoms must be within a specified "polyhedral distance range" of an atom in the ATOMS table which has an atom number satisfying a third atom number run, ANR(P). This option is brought into play by a negative number in columns 43 to 48 of the VSC card and is applicable to instructions 802, 803, 812, and 813.

Instructions 801, 802, and 803 differ from 811, 812, and 813 only in the monitor output listing. The second group has no output except error messages. The first group lists: (1) plotter coordinates in inches, (2) scaled Cartesian coordinates (in inches) of atom before projection, and (3) triclinic crystal coordinates for the atoms of each bond. The interatomic bond distance in angstroms is also listed. If an atom of a bonded pair is out of bounds, a fault message (NG = 10) is printed on the monitor output. If the bond is hidden and cannot be drawn, fault message NG = 14 is printed. Fault NG = 13 signifies that an imaginary intersection was found with a bond radius larger than the ellipsoid semidimension.

3.3.9.1 Instructions 801 and 811, Explicit Stick Bonds. – The bonds are described with two atom designator codes for each bond. The atom designator codes go on the 801 card and on Format No. 1 trailer cards (see Table 2.1 for format). The two atom designator codes for a bond must be in adjacent fields, but blank fields can be inserted between the different bonds. Since there are seven fields available per card, it is a good idea to use only two, four, or six of them so that the card sequence within the instruction (other than first and last cards) will be unimportant. In addition, a Format No. 2 trailer card is required with the fields specified under column 801 in Table 3.1 properly filled in.

3.3.9.2 Instructions 802 and 812, Implicit Stick Bonds. – All parameters are input with Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the instruction number and look ahead (2).

3.3.9.3 Instructions 803 and 813, Implicit Line Bonds. – All parameters are input with Format No. 2 trailer cards (see Table 3.1). The centered symbol placed on a given atom will be the centered symbol whose calling number corresponds to the atom number modulo 10 (see Fig. 4.2).

The centered symbols drawn on the atomic sites by the 803/813 instructions may be made larger or smaller by redefining the SCAL2 factor, which is controlled by the 600 series of instructions (3.3.7).

3.3.9.4 Instructions 821 and 822, Overlap Elimination. See Section 3.3.14.

3.3.10 Label Plotting Instructions (900 Series). – The 900 series allows the user to plot general titles up to 72 characters in length, chemical symbols up to 6 characters long, bond length labels, and centered symbols. The bond length labels can have two decimal places before the decimal point and one, two, or three places after the decimal point. The 700 and 800 series instructions can plot chemical symbols and bond length labels, but it is often desirable to position certain labels individually with the 900 series.

General titles and bond length labels can be drawn either in perspective or parallel to the plane of the drawing. Chemical symbols and centered symbols are always drawn parallel to the plotter plane. Instructions 913 through 916 are for perspective lettering, and instructions 901 through 909 produce regular lettering.

Two vectors, the upright vector and the base-line vector, are needed to describe a lettering plane. In OR TEP the upright lettering vector is always parallel to the plane of the drawing. For perspective lettering the base-line vector is a general vector in three dimensions. In the nonperspective case the base-line vector is either along the projection of a general vector or along the vector (in the plane of the plotter) which is oriented with a 302 title rotation instruction (theta base line). If theta (set by 302) is zero, then the theta base-line vector is along the plotter positive x axis.

The exact center of the label is always referred to when specifying the position of the label. The program goes through the following steps to position the center point of the label onto the drawing. (1) A point $P1$ is found which is either the position of atom A or the mean of two atom positions (atom A and atom B). The atom A position is used if no atom designator exists in the atom B field of the instruction card. (2) A point $P2$ is found by (*a*) translating from $P1$ along the base-line vector for the distance specified by *parallel offset*, then (*b*) translating along the upright vector by the *perpendicular offset* distance. (3) A point $P3$ is found by projecting $P2$ onto the plane of the plotter. (4) If the x *edge reset* is >0, then x is reset to this value. If x *edge reset* is <0, x is reset to the positive x plot boundary minus $|x$ *edge reset*$|$. No resetting is done if x *edge reset* is zero. The y parameter is handled in the same manner with y *edge reset*.

The format for the entire 900 series is as follows:

Columns	
1–3	Blank or 3 (or 1 if second card is needed)
4–9	Instruction number
10–18	Designator for atom A
19–27	Designator for atom B (or blank)
28–36	*x* edge reset (in.)
37–45	*y* edge reset (in.)
46–54	Lettering height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
	Second Card (if needed)
1–3	Blank
4–9	Blank
10–18	Centered symbol number (0–14)

3.3.10.1 Instruction 901. – A nonperspective chemical symbol with theta base line is drawn using the chemical symbol for atom A.

3.3.10.2 Instruction 902. – A nonperspective title with theta base line is drawn. The title must be entered with the instructions on a Format No. 3 trailer card. The title should be centered about columns 36–37 of that card.

3.3.10.3 Instructions 903 and 913. – A general vector title is drawn with nonperspective lettering for 903 and perspective lettering for 913. The general vector is from atom A to atom B. The title is entered as described for 902 (see 3.3.10.2 above).

3.3.10.4. Instructions 904, 905, 906, 914, 915, and 916. – These are instructions for general-vector bond-length labels. The first three are for nonperspective lettering with one, two, and three places after the decimal point; and the last three are for the corresponding bond-length labels with perspective lettering. The general vector is from atom A to atom B. Note that the sense of the vector is important in order to have the label right side up.

3.3.10.5 Instructions 908 and 909. – These instructions are for centered symbols. With 908 the pen is up while moving to the position where the centered symbol is to be drawn, but *with 909 the pen is left down.* The centered symbol is one of the 15 listed for the CalComp SIMBOL routine (the misspelling of "symbol" is intentional). The symbol number must be in the range 0–14.

3.3.11 Saved Sequence Instructions (1100 Series). – It is often desirable to repeat a sequence of instructions one or more times with other instructions inserted between the repetitions. The 1100 series allows the user to do this without the necessity of putting in duplicate sequences of instruction cards. It is not an elaborate looping device, but it does give additional flexibility to the system.

The three instructions in this series are to start the saved sequence (instruction 1101), terminate the saved sequence (instruction 1102), and execute the saved sequence (instruction 1103). All instruction

cards and their trailer cards between the 1101 and 1102 instructions are executed and saved on a magnetic scratch tape. A 1103 instruction rewinds this scratch tape and repeats all the instructions stored there before another instruction is read from the monitor input. There are no parameters to be entered with the 1100 series instructions.

3.3.12 Job Termination Instructions (Negative Series). – A (–1) instruction terminates the job and exits via SUBROUTINE EXIT.

A (–2) instruction reinitializes the whole program and starts over with another structure from the title card on. As many structures as desired may be run in sequence in this manner before exiting with a (–1) instruction. Note that the 201 instructions should occur only once and should not be repeated for succeeding jobs.

3.3.13 Supplementary Instructions (1200 Series). – These instructions utilize Subroutine SPARE.

3.3.13.1 Punching Cards with OR FLS Format. – An instruction 1201, which is implemented in subroutine SPARE, punches new position cards and temperature-factor cards with the format used by the OR FLS least-squares program. The instruction is useful for transforming a structure to a different asymmetric unit and for saving key atoms from a complex ATOMS array. First an ATOMS array is generated by the 400 series of instructions; then positional parameter cards, taken from the input atoms list, are read to define which atoms are wanted and to supply information about the scattering factor identifier and the multiplier. The parameter cards for all atoms in the ATOMS list which are crystallographically equivalent to the ones read are punched out. The sequence of the parameter cards read by this instruction need not correspond with the sequence of the original input atoms.

Columns

1–3 Blank

4–9 1201

10–18 *n* (the number of positional parameter cards to be read; *n* position parameter cards from the original input atom deck must follow this instruction card.)

3.3.14 Overlap Correction Instructions (511, 821, 822). – The hidden line correction feature of OR TEP-II eliminates most of the manual touch-up tasks previously required to correct for overlapping atoms and bonds. Drawings made with the overlap feature activated may require up to two or three times the computing time needed for noncorrected drawings; consequently, it is often more economical in computer time to make the preliminary drawings without overlap correction, particularly if a large number of atoms are present in the drawing.

To utilize the overlap feature an additional instruction, 511, is required, which is usually accompanied by type 2 trailer cards identical to those used by the 802 or 812 instructions. The 511 instruction stores the projected atom boundary ellipses for all atoms in the ATOMS list. It is important that the contents of the ATOMS list, the scaling and positioning, and the viewing parameters (controlled by the 400, 600, and 500 series of instructions respectively) not be changed between the 511 instruction and the drawing of the atoms and bonds by the 700 and 800 series of instruction; otherwise, the projected outlines may be destroyed or may be inappropriate.

The projected bond outlines, approximated as quadrangles, also may be stored for the overlap correction either by adding format No. 2 trailer cards to the 511 instruction or by using one or more 822 instructions (including those format No. 2 trailer cards) after the 511 instruction. The bonds to be stored are specified implicitly by the format No. 2 trailer cards. Explicit bonds also may be stored by using an 821 instruction (after the 511 instruction) with parameters identical to the 801/811 instructions to be used for plotting the explicit bonds.

The projected outline information for atoms and bonds must be recalculated for each member of a stereo pair; consequently the 511 and 821 or 822 instructions are usually the first instructions within the saved sequence. The old overlap information is removed whenever a new 500 or 600 series instruction is executed.

The maximum number of projected atoms and projected bonds which can be stored is 500 and 599 respectively. A list of the projected atoms and bonds is given in the printout.

An important feature of the OR TEP-II scheme for correcting overlap is that all details *inside* atoms and bonds, including chemical symbols and bond-distance labels, will be corrected for overlap; however, note that chemical symbols (drawn by the 700 series instructions and bond-distance labels (drawn by the 800 series instructions) which are *outside* the atoms or bond boundary *may not be corrected* for overlap. The reason for this is that the "area overlap search step" does not save projected atoms or bonds which do not contact the projected atom or bond to be drawn. Labels or symbols drawn with the 900 series instructions will not be corrected for overlap.

3.3.14.1 Instruction 511, Projected Outline Storage. – A constant width overlap margin (i.e., a blank strip at the intersection of overlapping elements) is included in the dimensions of each projected atom ellipse and projected bond quadrangle. The width of this margin may be specified as a parameter with the 511 instruction if desired; otherwise, the margin is set by default to either 0.025 inch or $(\mathrm{SCAL1})^{1/2} \times 0.030$ inch, whichever is largest. Some users prefer an overlap margin of 0.0 for stereoscopic drawings.

Columns	
1–3	2 (if bonds are to be stored; otherwise 0)
4–9	511
10–18	Blank or 0 – overlap margin default option described above 1 (or –1) – overlap margin = 0.0 $0 < \mathrm{OVMRGN} < 1.0$ – overlap margin = OVMRGN (in inches)

If column 3 is 2, format no. 2 trailer cards are included. In general all the trailer cards included with the 802/812 instructions are used.

3.3.14.2 Instruction 821, Explicit Bond Outline Storage. – If explicit bonds are to be stored for the overlap calculation, the attached atoms must be in the ATOMS list even though this is not a requirement for the 801/811 instructions used for plotting the explicit bonds. See 3.3.9.1 (Instructions 801 and 811) and Table 3.1 for description of parameters.

3.3.14.3 Instruction 822, Implicit Bond Outline Storage. – Normally the information on implicit bond outlines is stored with the 511 card; however, if more than 10 Format No. 2 trailer cards are needed, the extra ones can be entered with this instruction. All parameters are entered with the Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the 2 in column 3 and 822 in columns 7–9.

3.4 List of Fault Indicators

Certain errors are checked for in OR TEP, and when one of these occurs, an error message, "FAULT NG = *ng ADC m*" is written on the monitor output tape. The number NG is explained below. The *ADC* and *m* identify the atom code and the instruction involved (if these are relevant). If possible, corrective measures are made by OR TEP and the calculation proceeds; otherwise, the job is terminated by calling SUBROUTINE EXIT.

NG	Subroutine Involved	Fault	Action
1	PRELIM	No sentinel found after reading 48 symmetry cards	Tries to read parameter cards
2	PRELIM	No sentinel found after reading the parameter cards for 100 atoms	Tries to read instruction cards
3	PRELIM	Anisotropic temperature factor coefficients form a matrix which is not positive definite	EXIT after printing out all rms principal values (imaginary ones are listed negative)
4	ATOM,PAXES	Symmetry operation number is higher than the number of input operations	Omit atom
5	ATOM,PAXES	Atom number is higher than the number of input atoms	Omit atom
6	EIGEN	Null temperature factor matrix or failure in bisection routine	EXIT, after printing out all principal values
7	EIGEN	Eigenvector routine failure due to null vector	EXIT, after printing out all principal values
9	MAIN,SPARE	Unidentified instruction number	Omit faulty instruction
10	BOND,F700	Atom out of bounds	Omit atom
11	F800	No vector search codes	Omit instruction
12	F600, SEARCH	Insufficient number of atoms in ATOMS list	EXIT
13	BOND	Imaginary bond intersection (i.e., bond larger than atom)	Omit bond
14	BOND	Hidden (end-on) bond	Omit bond
15	F900	Null vector as base line	Omit label
16	STORE	ATOMS list is full	Omit all succeeding atoms

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

Certain of the numerical procedures[1] used in OR TEP are of a nature somewhat unfamiliar to many crystallographers. These aspects are outlined for the benefit of the reader who may wish to write a similar program or modify the present one.

4.1 Graphic-Computational Methods

These are the techniques used in producing the graphical details of the illustrations.

4.1.1 Drawing Ellipsoids. – Figure 3.1 demonstrates the various ellipsoid graphical representations that can be drawn with OR TEP. The major components in the representations are the three principal ellipses and the boundary (outline) ellipse. The principal ellipses have a front half and a back (hidden) half. The entire boundary ellipse is visible.

An ellipse is approximated by connecting a series of points on the ellipse with straight line segments. Points on an ellipse having a general orientation in three dimensions are computed; then each of these points is projected onto the drawing board for plotting.

The basic algorithm for finding the points along a given general ellipse utilizes the properties of conjugate diameters. Assume that we have the three principal axis vectors **V1**, **V2**, **V3** of the general ellipsoid and a vector **V4** from the center of the ellipsoid to the viewpoint. The vector **V5** normal to the polar plane (see Fig. 4.1), whose pole is the viewpoint, can be obtained from

$$\mathbf{V5} = \mathbf{A}\,\mathbf{V4}\ , \tag{4.1.1.1}$$

where **A** is the matrix for the ellipsoid which is defined by

$$\mathbf{X}^T\,\mathbf{A}\,\mathbf{X} = d\ , \tag{4.1.1.2}$$

where d is a constant.

The boundary ellipse is defined by two conjugate vectors, one of which is any vector **V6** perpendicular to **V5** and the second is **V7**, where

$$\mathbf{V7} = \mathbf{V5} \times \mathbf{A}\,\mathbf{V6}\ . \tag{4.1.1.3}$$

The assumption made for this boundary ellipse derivation is that the view distance is large compared to the ellipsoid size. Therefore, the boundary ellipse defined above always lies on the diametral polar plane (see Fig. 4.1).

[1]For a treatment of the projective and analytical geometry involved, the following four books are recommended. The first one is particularly useful.

J. Heading, *Matrix. Theory for Physicists*, chap. 3, pp. 81–106, Longmans, Green and Co., London, 1958.

C. E. Springer, *Geometry and Analysis of Projective Spaces*, Freeman and Co., San Francisco, 1964.

J. A. Todd, *Projective and Analytical Geometry*, Pitman Pub. Corp., New York, 1946.

G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers*, McGraw-Hill Book Company, New York, 1961.

ORNL-DWG. 65-2671

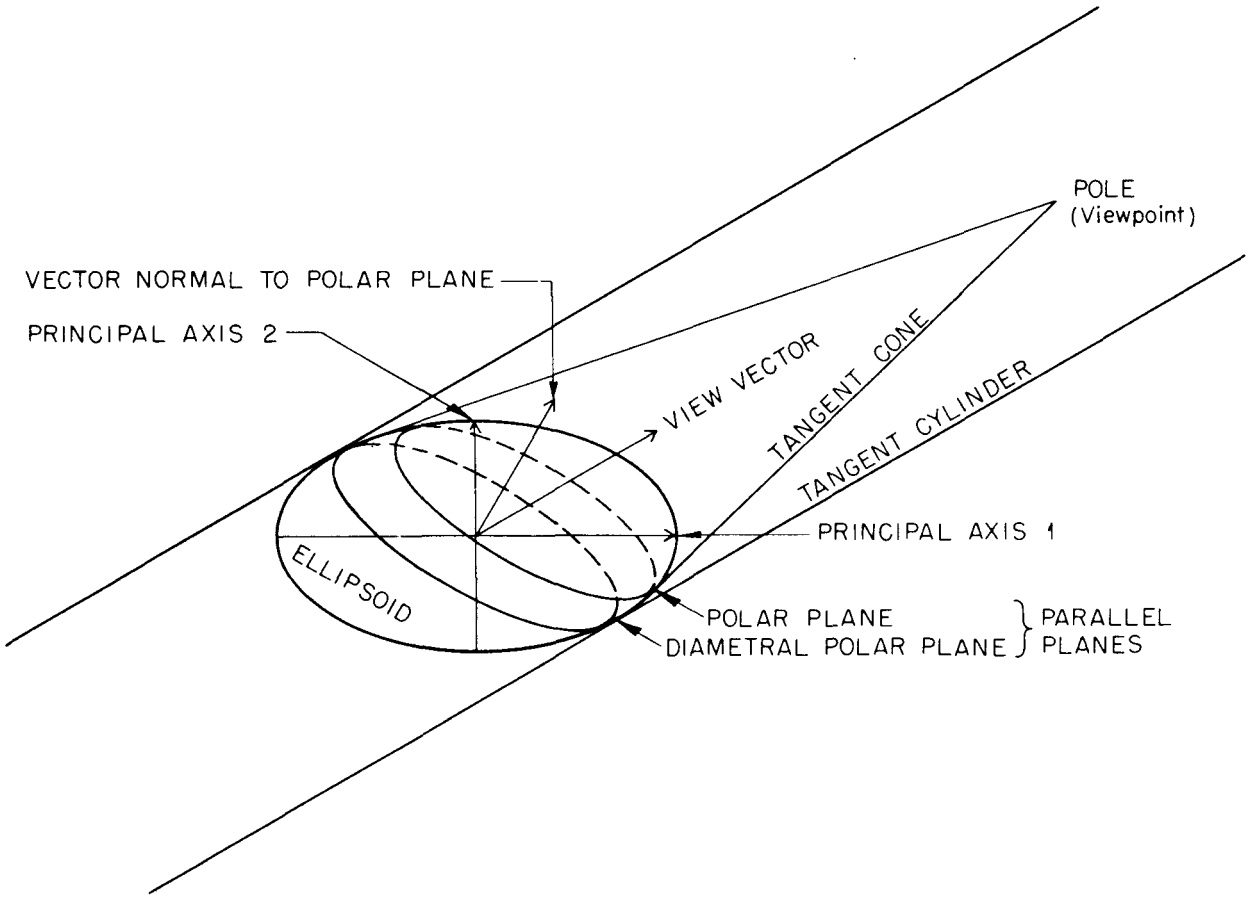

Fig. 4.1. Polar Planes Formed by Tangent Cylinder and Tangent Cone.

A principal ellipse which lies in the plane of the principal axis vectors **V1** and **V2** will have the third principal axis vector **V3** normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector **V8** where

$$\mathbf{V8} = \mathbf{V5} \times \mathbf{V3} \ . \tag{4.1.1.4}$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to **V8** and in the principal plane containing **V1** and **V2** is **V9**, where

$$\mathbf{V9} = \mathbf{V3} \times \mathbf{A}\,\mathbf{V8} \ . \tag{4.1.1.5}$$

After the conjugate vectors have been found, their lengths are adjusted to make them satisfy (4.1.1.2) by letting $\mathbf{X} = s\,\mathbf{l}$ where $\mathbf{l}$ is a unit vector. Solving for s, we obtain

$$s = [d/(\mathbf{l}^T \mathbf{A}\,\mathbf{l})]^{1/2} \ . \tag{4.1.1.6}$$

A conjugate vector pair is expanded into an ellipse by subroutine RADIAL. Since an ellipse is centrosymmetric, the two conjugate vectors and their negatives give us four vectors whose end points lie on the ellipse. By performing a vector sum of two adjacent vectors and dividing the resultant vector components by $\sqrt{2}$, we can obtain an additional vector. After doing this for all adjacent pairs, we then have a total of eight vectors. This process can be repeated as many times as desired except that the scaling constant will be different for each cycle. The constant is described by

$$\mathrm{CONT}\,(i) = \{2[1 + \cos\,(\pi/2^i)]\}^{1/2} = 2\cos\,(\pi/2^{i+1})$$

where i is the cycle number.

This total process may be thought of as taking a planar radial set of equally spaced unit vectors and performing a deformation and scaling on the space in which it is described. In geometry this deformation is called an affine transformation.

Complete details on drawing ellipsoids can be obtained from the FORTRAN coding of subroutines F700 and RADIAL.

4.1.2 Drawing Bonds. – The major problem in drawing bonds is to obtain the intersection where the bond penetrates the ellipsoid. Three quadrics are used in subroutine BOND to calculate bond intersection. These three are the ellipsoid, the tangent cylinder, and the tangent cone.

The ellipsoid is described in matrix notation as

$$\mathbf{X}^T\mathbf{A}\,\mathbf{X} = d\,, \tag{4.1.2.1}$$

where d is a constant and $\mathbf{X}$ is any vector from the center to the surface of the ellipsoid. The matrix $\mathbf{A}$ is 3 by 3 symmetrical with components a_{ij} $(i,j = 1, 2, 3)$.

The elliptic cylinder tangent to the ellipsoid and with its axis along z is described by

$$\mathbf{X}^T\mathbf{B}\,\mathbf{X} = d\,, \tag{4.1.2.2}$$

where

$$\mathbf{B} = \begin{pmatrix} a_{11} - \dfrac{a_{13}a_{31}}{a_{33}} & a_{12} - \dfrac{a_{23}a_{31}}{a_{33}} & 0 \\ a_{12} - \dfrac{a_{13}a_{32}}{a_{33}} & a_{22} - \dfrac{a_{23}a_{32}}{a_{33}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.1.2.3}$$

and d is the constant used in (4.1.2.1). The tangent cylinder is used when it is necessary to terminate the bond at the boundary of the ellipsoid *when a parallel projection is used.*

To find the intersection of a cylindrical bond along $\mathbf{Vb}$ with radius r with either the ellipsoid or the tangent cylinder, we proceed as follows:

1. Form a radial set of vectors $\mathbf{Vr}_j$ of length r normal to $\mathbf{Vb}$.

2. Take a unit vector **l** parallel to **Vb** and let

$$\mathbf{X}_j = \mathbf{Vr}_j + s\,\mathbf{l}\,, \tag{4.1.2.4}$$

where s is a constant to be determined. Substituting in (4.1.2.1) we obtain

$$s^2 \mathbf{l}^T \mathbf{A}\,\mathbf{l} + 2s\,\mathbf{Vr}^T \mathbf{A}\,\mathbf{l} + \mathbf{Vr}^T \mathbf{A}\,\mathbf{Vr} - d = 0\,; \tag{4.1.2.5}$$

solving for s we get

$$s = \frac{-\mathbf{Vr}^T \mathbf{A}\,\mathbf{l} + \sqrt{(\mathbf{Vr}^T \mathbf{A}\,\mathbf{l})^2 - (\mathbf{l}^T \mathbf{A}\,\mathbf{l})(\mathbf{Vr}^T \mathbf{A}\,\mathbf{Vr} - d)}}{\mathbf{l}^T \mathbf{A}\,\mathbf{l}}\,. \tag{4.1.2.6}$$

The elliptic cone which is tangent to the ellipsoid and which has its apex on the viewpoint can be obtained from the matrix **A** and from the vector **Vu** which extends from the center of the ellipsoid to the viewpoint. This is performed in the following steps:

1. The ellipsoid is transformed with a rotation matrix to a new Cartesian frame of reference which has the z axis along the view vector **Vu**.
2. The tangent cone can now be described as

$$\mathbf{Y}^T \mathbf{C}\,\mathbf{Y} = 0\,, \tag{4.1.2.7}$$

where **Y** is a vector originating from the vertex (viewpoint) of the cone and

$$\mathbf{C} = \begin{pmatrix} a_{11} + \dfrac{a_{13}a_{31}}{K - a_{33}} & a_{12} + \dfrac{a_{13}a_{32}}{K - a_{33}} & \dfrac{Ka_{13}}{K - a_{33}} \\ a_{21} + \dfrac{a_{23}a_{31}}{K - a_{33}} & a_{22} + \dfrac{a_{23}a_{32}}{K - a_{33}} & \dfrac{Ka_{23}}{K - a_{33}} \\ \dfrac{Ka_{31}}{K - a_{33}} & \dfrac{Ka_{32}}{K - a_{33}} & \dfrac{Ka_{33}}{K - a_{33}} \end{pmatrix}, \quad K = d/(\mathbf{Vu}^T \mathbf{Vu}). \tag{4.1.2.8}$$

3. The frame of reference is rotated back to its original orientation with a rotation matrix which is the inverse of the one used in step 1. Note that the origin is now on the viewpoint rather than the ellipsoid center.

To find the length, s, of a vector $s\,\mathbf{l}$ extending from any point p inside the cone to the surface of the cone we let

$$\mathbf{Y} = \mathbf{Vp} + s\,\mathbf{l} \tag{4.1.2.9}$$

and obtain from (4.1.2.7)

$$(\mathbf{Vp} + s\,\mathbf{l})^T\,\mathbf{C}\,(\mathbf{Vp} + s\,\mathbf{l}) = 0\,;$$

then solving for s we obtain

$$s = \frac{-\mathbf{V_p}^T \mathbf{C}\,\mathbf{l} + \sqrt{(\mathbf{V_p}^T \mathbf{C}\,\mathbf{l})^2 - (\mathbf{l}^T \mathbf{C}\,\mathbf{l})(\mathbf{V_p}^T \mathbf{C}\,\mathbf{V_p})}}{\mathbf{l}^T \mathbf{C}\,\mathbf{l}} \tag{4.1.2.10}$$

The vector $\mathbf{V_p}$ from the vertex to $\mathbf{p}$ is formed by

$$\mathbf{V_p} = -\mathbf{V_u} + \mathbf{V_r} ,$$

where $\mathbf{V_r}$ is any member of a radial set such as that described for the regular ellipsoid intersection.

4.2 OR TEP Subprograms

The subprograms can be grouped into four functional categories. These can be called Mainstream, Subsidiaries, Arithmetic, and Plotting. The first three categories are coded in a FORTRAN dialect which will compile with either IBM-7090 FORTRAN II or CDC-1604A FORTRAN 63. The plotting routines are generally different for each machine configuration and are usually written in a machine-oriented symbolic language. In general, the standard library plotting routines available at most computing centers can be used with very minor modification.

4.2.1 Mainstream Subprograms. – The first three (PRIME, PRELIM, and MAIN) are the general controlling routines, and the remainder are oriented toward particular OR TEP instructions.

4.2.1.1 PRIME. – This routine "primes the program" by initializing all the "primer parameters" including the magnetic tape logical number assignments.

4.2.1.2 PRELIM. – All calculations concerned with processing (e.g., principal axis transformations) and storing the input crystallographic parameters are performed by PRELIM.

4.2.1.3 MAIN. – MAIN is the controlling routine which decodes the OR TEP instructions. It either executes the command directly or calls the appropriate subroutine which can execute the instruction.

4.2.1.4 F200. – This is the plotter "nursemaid routine" which is controlled through the 200 series instructions. It satisfies the whims and fancies of any particular plotting system control package.

4.2.1.5 F400. – This is the subroutine that executes the 401 and 411 instructions.

4.2.1.6 F500. – This is the subroutine that executes all 500 series instructions.

4.2.1.7 F600. – This is the subroutine that executes all 600 series instructions.

4.2.1.8 F700. – This is the ellipsoid plotting routine, which executes all 700 series instructions.

4.2.1.9 F800. – This is the subroutine that executes all 800 series instructions. Bonds to be drawn are found by F800, then drawn by subroutine BOND.

4.2.1.10 F900. – This is the subroutine that executes all 900 series instructions.

4.2.1.11 F1000. – This is a dummy subroutine which is called by the presently nonexistent 1000 series instructions. This series can be coded by the user for any special purpose which may develop.

4.2.1.12 SPARE(NJ). – Further expansion of the instruction list may be done through this dummy subroutine, which is called by any $NJ \geqq 12$. NJ = instruction/100.

4.2.2 Subsidiary Subprograms. – **4.2.2.1 ATOM(ADC,X),** DIMENSION X(3). – This will find the triclinic coordinates **X** for the atom described by the atom designator code ADC.

4.2.2.2 BOND (ADC1, ADC2, NB). – BOND is the bond plotting routine to draw a bond, described by Format No. 2 trailer card number NB, between atoms ADC1 and ADC2.

4.2.2.3 DRAW (W,DX,DY,NPEN), DIMENSION W(3). – DRAW interconnects OR TEP and the plot package. It also prevents the pen from crossing the boundaries. If the indicator ITILT in common is zero, the array W contains x and y in plotter coordinates. While perspective lettering is being plotted, ITILT $\neq 0$; and W contains x, y, z in Cartesian coordinates, which will be rotated and projected by DRAW to form plotter x,y coordinates. DX and DY are added to the plotter x and y, respectively, before the plot package is called. NPEN = 2 for pen down and 3 for pen up.

4.2.2.4 ERPNT (ADC,INST). – This is the printout routine called when a Fault is found. The arguments identify the atom designator code and the instruction involved in the Fault. The fault indicator, NG, is in common.

4.2.2.5 PAXES (ADC,ITYPE). – The covariance (dispersion) matrix for the thermal ellipsoid or its inverse matrix, which is the matrix of coefficients in the quadratic form describing the ellipsoid, is stored in common at Q for the atom ADC.

ITYPE > 0 for covariance matrix

ITYPE < 0 for ellipsoid quadratic form matrix

$|$ITYPE$|$ = 1 based on triclinic system

$|$ITYPE$|$ = 2 based on working Cartesian system

$|$ITYPE$|$ = 3 based on reference Cartesian system

4.2.2.6 PLTXY (X,Y), DIMENSION X(3),Y(2). – This calculates the plotter coordinates Y from the unscaled Cartesian coordinates X. The distance to the closest boundary of the plot is placed in common at location EDGE.

4.2.2.7 PROJ (D,DP,X,XO,VIEW,I1,I2,I3), DIMENSION D(3,129),DP(2,129),X(3),XO(3). – This routine is used to obtain an array, DP, of plotter coordinates from a scaled array, D, of points described in Cartesian coordinates. X, XO, and VIEW are parameters involved in the projection, and I1, I2, I3 are DO loop parameters for indexing through the array.

4.2.2.8 RADIAL(ND). – Given two conjugate radius vectors of an ellipse in the array DA in common, RADIAL generates a "radial" array (D in common) of points lying on the ellipse. From 8 to 128 points are generated depending on the value of ND ($1 \leqq$ ND $\leqq 5$).

4.2.2.9 SEARCH. – Instructions 101, 102, 402, and 403 utilize this routine to conduct an exhaustive (but educated) search to find all points within a sphere or rectangular box. Interatomic distances and angles are also calculated for the 100 series.

4.2.2.10 STORE. – This routine stores atoms in (or removes atoms from) the ATOMS array. Coordinates in whichever system is in use and the atom designator code are communicated to STORE via array V1 of common.

4.2.2.11 XYZ(ADC,X,ITYPE), DIMENSION X(3). – Coordinates for atom ADC are returned in X.

ITYPE = 0: triclinic coordinates

ITYPE = 1 or 2: working Cartesian system coordinates

ITYPE = 3: reference Cartesian system coordinates

4.2.2.12 LAP500. – This routine sorts the ATOMS list, then calculates the projected outline ellipses for all atoms in the ATOMS list. The ellipses are stored in the CONIC array along with the minima and maxima in x and y for a rectangle enclosing each ellipse.

4.2.2.13 LAP700. – This routine finds the atoms which overlap a given atom to be drawn. The routine first checks the bounding rectangles for intersections, then forms the cubic discriminant from the quadratic descriptions of the two projection ellipses. The discriminant provides a specification for complete overlap, partial overlap or no overlap. A list of up to 20 interfering ellipses is compiled.

4.2.2.14 LAP800. – This routine is used in the "Projected Outline Storage Step" to store the projected quadrangles for the bonds specified by the trailer cards of the 511, 821, and 822 instructions. The routine also is used in the "Area–Overlap Search Step" to find the projected bond quadrangles which overlap a given bond to be drawn. A list containing up to thirty interfering quadrangles is compiled.

4.2.2.15 LAPAB. – This routine finds the bonds that overlap an atom to be drawn and the atoms that overlap a bond to be drawn. It is used in the "Area–Overlap Search Step."

4.2.2.15 LAPDRW. – This routine checks each line segment to be drawn for intersection with the interfering ellipses and quadrangles and compiles a list of intersections. The intersection list is sorted according to distance along the line segment, and the intersection pattern is analyzed to determine which subsegments are visible and which are hidden. The line subsegments are passed to the SCRIBE routine.

4.2.2.17 SCRIBE. – This routine filters out the hidden line segments and passes the visible line segments to the DRAW routine.

4.2.3 Arithmetic Subprograms. – 4.2.3.1 Function ARCCOS (X). – This routine computes θ, the arc cosine of X in degrees; $0 \leqq \theta \leqq 180°$.

4.2.3.2 AXEQB (A,X,B,N), DIMENSION A(3,3),X(3,3),B(3,3). – This routine solves the matrix equation $\mathbf{A}\,\mathbf{X} = \mathbf{B}$ for $\mathbf{X}$. The matrices $\mathbf{B}$ and $\mathbf{X}$ are (3,N) and $\mathbf{A}$ is always (3,3). To invert $\mathbf{A}$, make $\mathbf{B}$ an identity matrix.

4.2.3.3 AXES (X, Y, A, ITYPE), DIMENSION X(3),Y(3),A(3,3). – This routine provides three orthogonal column vectors in $\mathbf{A}$, each 1 A long, from the two vectors $\mathbf{X}$ and $\mathbf{Y}$.

ITYPE > 0: Cartesian system

ITYPE $\leqq 0$: triclinic system

$|\text{ITYPE}| = 1$: $\mathbf{A}_1 = \mathbf{X}$; $\mathbf{A}_2 = (\mathbf{X} \times \mathbf{Y})$; $\mathbf{A}_3 = \mathbf{X} \times (\mathbf{X} \times \mathbf{Y})$

$|\text{ITYPE}| = 2$: $\mathbf{A}_1 = \mathbf{X}$; $\mathbf{A}_2 = (\mathbf{X} \times \mathbf{Y}) \times \mathbf{X}$; $\mathbf{A}_3 = \mathbf{X} \times \mathbf{Y}$

ITYPE $= 0$: same as type 2 except $\mathbf{X} = a$ crystal axis, $\mathbf{Y} = b$ crystal axis.

4.2.3.4 DIFV (X,Y,Z), DIMENSION X(3),Y(3),Z(3). – This routine performs the vector subtraction $\mathbf{X} - \mathbf{Y} = \mathbf{Z}$. $\mathbf{Z}$ may have the same location as $\mathbf{X}$ or $\mathbf{Y}$.

4.2.3.5 EIGEN (A,X,B), DIMENSION A(3,3),X(3),B(3,3). – EIGEN determines the three eigenvalues $\mathbf{X}$ and the three column eigenvectors $\mathbf{B}$ of the matrix $\mathbf{A}$. Indeterminate eigenvectors are replaced by zeros and the Fault indicator NG set to a negative value (eigenvectors are assigned for the indeterminate cases by PRELIM).

4.2.3.6 MM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3). – MM performs the matrix multiplication **A B** = **C**. The location of **C** must be different from **A** and **B**.

4.2.3.7 MV (A,X,Y), DIMENSION A(3,3),X(3),Y(3). – MV performs the matrix-vector multiplication **A X** = **Y**. The location of **Y** must be different from **A** and **X**.

4.2.3.8 NORM (X,Y,Z,ITYPE), DIMENSION X(3),Y(3),Z(3). – NORM stores at **Z** a vector (not necessarily a unit vector) perpendicular to both **X** and **Y**. The sense of **Z** is that of the vector product **X** × **Y**.

ITYPE > 0: Cartesian system

ITYPE ≦ 0: triclinic system

4.2.3.9 TMM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3). – TMM performs the matrix multiplication $(\mathbf{A}^T\ \mathbf{B})^T = \mathbf{C}$. The location of **C** must be different from **A** and **B**.

4.2.3.10 UNIT (X,Y,ITYPE), DIMENSION X(3),Y(3). – The vector **Y** is made 1 A long and parallel to **X**. The vectors **X** and **Y** may have the same location.

ITYPE > 0: Cartesian system

ITYPE < 0: triclinic system

4.2.3.11 VM (X,A,Y), DIMENSION X(3),A(3,3),Y(3). – VM performs the vector-matrix multiplication $\mathbf{X}^T\mathbf{A} = \mathbf{Y}^T$. The location of **Y** must be different from **X** and **A**.

4.2.3.12 FUNCTION VMV (X,A,Y), DIMENSION X(3),A(3,3),Y(3). – VMV performs the vector-matrix-vector multiplication $\mathbf{X}^T\mathbf{A}\ \mathbf{Y}$ = scalar.

4.2.3.13 FUNCTION VV (X,Y), DIMENSION X(3),Y(3). – VV performs the vector-vector multiplication $\mathbf{X}^T\mathbf{Y}$ = scalar.

4.2.4 Plotting Subprograms for the CalComp Plotter. – The plotting subroutines are taken from the Library routines currently in use at Oak Ridge National Laboratory with the CDC 1604A and the IBM 7090 computers. A CalComp model 580 Magnetic Tape Plotting System is used. The three major routines required are derived from the CalComp subroutines PLOTS, SYMBOL, and NUMBER. The OR TEP modifications are called PLOTS, SIMBOL, and NUMBUR.

4.2.4.1 Subroutine PLOTS. – This is an unmodified CalComp Library routine with two entry points.

a) ENTRY – PLOTS (A, LENGTH, LTNO)

This is the initialization entry for the plotter package and should be used only once in the program. This call must be made prior to usage of any other subroutines in the package.

A is an array which may be used by the plotting package for storing data to be written on the plot tape.

LENGTH is the number of locations in A available to the plotter package.

LTNO is an integer which tells the plotter package the logical tape number of the plotter tape.

In subroutine F200 we have

DIMENSION PLA(1500)

and card F2000180 contains

"210 CALL PLOTS (PLA,1500, LTNO)"

for the CDC 1604-A or

"210 CALL PLOTS (PLA(1500),1500,LTNO)"

for the IBM 7090. The reverse storage of common in the IBM 7090 is the reason for the difference. LTNO is in common and was set to 23 by subroutine PRIME.

An ORTEP 201 instruction directs the execution of this initialization.

b) ENTRY – PLOT (X,Y,IPEN)

This is the basic entry to convey data to the subroutine for plotting. To facilitate the substitution of other plotting routines, ORTEP contains only one instruction (card DRAW0330 in subroutine DRAW) which calls this entry point. All the plotting information passes through DRAW before going to the actual plotting routine PLOT.

X is the abscissa expressed in inches.

Y is the ordinate expressed in inches.

IPEN = 3, the pen will be lifted prior to execution of the movement to the given (**X**,**Y**) position.

IPEN = 2, the pen will be lowered to the paper and a straight line will be drawn from the current (**X**,**Y**) to the given (**X**,**Y**) position.

IPEN = –3, the subroutine will interpret this as being the end of the current plot; and, following movement to the new (**X**,**Y**) position, it will set **X** = 0.0, so that a new origin is established for the following plot (an ORTEP 202 instruction executes this termination procedure).

This subroutine keeps track of current **X** and **Y** positions, and whether or not the pen is in contact with the paper. It stores data in the array A provided by the programmer and writes out a record on the specified tape each time the storage area is filled or an end-of-plot call is made. It also generates sequential plot addresses for each plot on the magnetic tape, so that physical plotting of the plots can be done in any order, regardless of the order in which they were placed on tape.

4.2.4.2 Subroutine SIMBOL. – SIMBOL differs from the standard routine SYMBOL in two respects:

1. The input positional parameters specified in the input argument should be an array containing *X*, *Y*, and *Z* in adjacent memory locations. Three-dimensional parameters are required to produce perspective labels. The *Z* parameter is not used by SIMBOL but is transferred to another array that is referenced when SIMBOL calls DRAW.

2. The standard routine SYMBOL calls PLOT directly while SIMBOL calls DRAW which in turn calls PLOT. When perspective labels are used, DRAW will perform a three-dimensional rotation and a projection of the grid points on which the letters are formed, to obtain true perspective. The calling sequence for DRAW is described in 4.2.2.3.

There are two uses of subroutine SIMBOL. The first use is for producing labels, and the second is for plotting one of 15 special centered symbols.

1. ENTRY – SIMBOL (X(1),X(2),H,BCD,THETA,N), DIMENSION X(3) (note $N \geqq 0$)

   X(1),X(2) are the X and Y coordinates of the lower left-hand edge of the first character to be drawn.

   X(3) is the Z coordinate. It is used only with perspective labeling.

   H is the height in inches of the character to be drawn. The width of the character is equal to $^4/_7$ the height and the character spacing is $^6/_7$ the height.

   BCD specifies the address of an array containing the BCD characters to be plotted.

   THETA is the angle in degrees by which the base line of the characters is to be rotated counterclockwise from the positive X axis.

   N is an integer which specifies the number of characters in the array BCD that are to be drawn.

2. ENTRY – SIMBOL (X(1),X(2),H,NUM,THETA,L), DIMENSION X(3) (note $L < 0$)

   X(1),X(2) are the X and Y coordinates of the center of the symbol.

   H is the height of the symbol to be plotted.

   NUM is an integer such that $0 \leqq NUM \leqq 14$ which determines which symbol is to be plotted. A list of the integers and the symbols generated is shown in Fig. 4.2.

   THETA is the angle of rotation as described previously.

   $L = -1$: the centered symbol will be plotted without a line being drawn from the previous (X,Y) position.

   $L < -1$: a straight line will be drawn from the previous (X,Y) position to the given (X,Y) position.

4.2.4.3 Subroutine NUMBUR. – This is a subroutine to convert a machine format number to its BCD equivalent and plot it according to a specified format.

NUMBUR is different from the usual subroutine NUMBER in that it calls SIMBOL rather than SYMBOL.

ENTRY – NUMBUR(X(1),X(2),H,A,THETA,N)

X(1),X(2),H and THETA are described in Sect. 1 of the SIMBOL routine

A is the address of the floating or fixed point number which is to be plotted.

N is the number of digits to the right of the decimal point. A(–1) value will suppress the decimal point.

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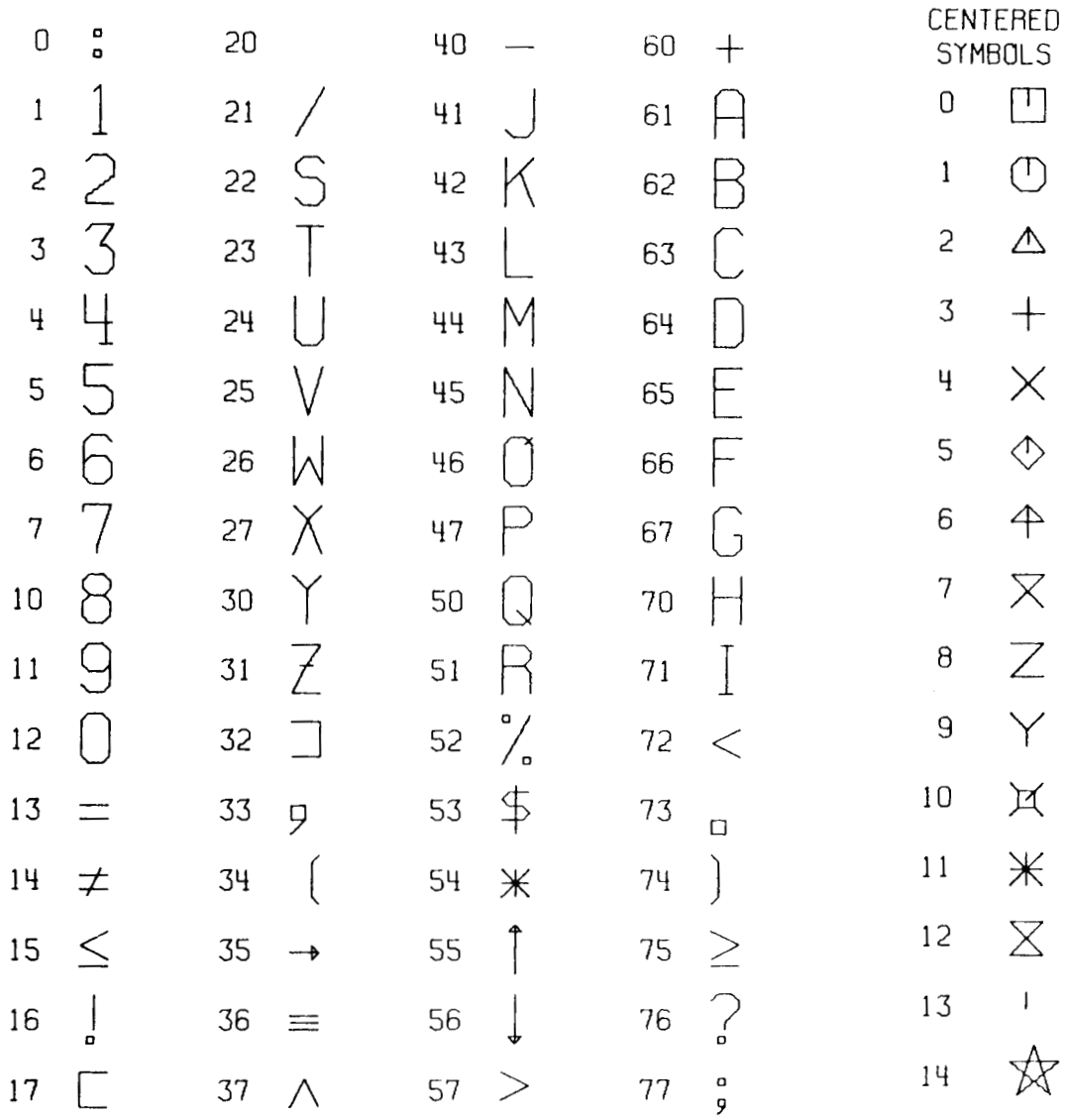

Fig. 4.2. Characters Available in 1604-A Symbol Routine.

4.3 Adapting OR TEP to Other Equipment Configurations

Card images[2] for OR TEP will be provided to crystallographers and others who request that the program be sent to them.

FORTRAN decks are available in IBM 360 FORTRAN IV and IBM 7090 FORTRAN IV. The FORTRAN subprograms are arranged alphabetically within the FORTRAN source decks. An exception is MAIN, which is first in each deck.

[2]The size of the card deck (3000–6000 cards) is such that it is generally more economical to send the program on magnetic tape. If convenient, the user should send a blank magnetic tape to the author. Card images will be written on that tape in an agreed upon format and the tape returned to the sender.

The machine language subroutines SIMBOL and NUMBUR are modifications of the CalComp subroutines SYMBOL and NUMBER. Subroutine PLOT is an unmodified CalComp subroutine also written in machine language. These three subroutines are copyrighted by California Computer Products, Inc. Subroutines SIMBOL and NUMBUR for IBM 360, IBM 7090, and CDC 1604-A can be distributed from ORNL. Subroutine PLOT which is different for each plotter may be obtained from California Computer Products, Inc., 305 Muller Avenue, Anaheim, California (Attention: Programming Dept.).

Cards for the example figure, cubane, will be included with the deck.

4.3.1 OR TEP Source Deck Differences for the IBM 360 and the IBM 7090. – The listing of the FORTRAN IV source deck for the IBM 360 is given in Sect. 7. The length of the single-precision floating-point word in the IBM 360 is such that the maximum number of atoms in the input list cannot be greater than 166 because of the way the atom designators are stored. This must be taken into account if the dimension statements of the program are changed.

The following changes are made to modify the program for IBM 7090 FORTRAN IV:

1. Remove the "REAL*8 CHEM" card from the subprograms which use common.
2. Add the correct IBSYS monitor control cards including "$POOL" and "$GROUP" cards to conserve memory space.

The following changes are made to modify the program for IBM 7090 FORTRAN II:

1. Remove the "REAL*8 CHEM" cards from the subprograms which use common.
2. Add "*LIST8" and "*LABEL" cards before each subprogram.
3. Replace card F2000180 with "210 CALL PLOTS (PLA(1500), 1500,LTNO)."
4. Change input-output statements and library function names to correspond with FORTRAN II convention.

4.3.2 External Device Logical Number Assignments. – Logical device number assignments are made in subroutine PRIME. Four cards are involved in this initialization:

Magnetic Tape Function	Symbolic Name		Primer Constant	Location in PRIME
a) Monitor Input	IN	=	5	PRIM0220
b) Monitor Output	NOUT	=	6	PRIM0280
c) Scratch	NSR	=	8	PRIM0290
d) Plotting	LTNO	=	23	(PRIM0250)*

4.3.3 Plotter Systems Other than the CalComp 580. – In general, only subroutine PLOTS (with entries PLOTS and PLOT) needs to be replaced when a different plotting system is used. This routine is called from only two locations, one in F200 and the other in DRAW. F200 will probably have to be rewritten, and

*In the present revision, LTNO also serves as a plotting device indicator and is initialized to zero at MAIN0145. For the mechanical plotter (CRT), LTNO is set to 15 (–99) at F2000210 (F200250) by a 201 (203) instruction.

the 200 series instructions may have to be redefined and expanded to accommodate the rules of the new system.

Location DRAW0330 in subroutine DRAW should also be modified to call the new line-drawing routine with the correct argument.

4.3.4 Computing Systems Other Than the IBM 360, IBM 7090, and CDC 1604-A. – Basically, the OR TEP system is designed to be used in a 32 K memory. Consequently, OR TEP would have to be changed considerably to operate in a much smaller memory.

The FORTRAN coding of OR TEP has proven to be fairly machine independent, but as compilers become more sophisticated new problems continually appear. For example, some compilers rearrange the sequence of operations to obtain more efficient execution and sometimes they "outsmart" themselves in the process. Certain of the 6000 series CDC compilers occasionally take an instruction such as I1 = ATOMS(1, J) / 100000. and make it into TEMP = 1./100000.; I1 = ATOMS(1,J)*TEMP. The effect is disastrous because the numerical rounding and truncation produce an incorrect integer I1.

If it becomes necessary to replace the machine language subroutines SIMBOL and NUMBUR with completely different routines, the statements calling these routines will also need to be modified.

SIMBOL is called from BOND0460, BOND0480, F7000850, F9001310, F9001340, and F9001470.

NUMBUR is called from BOND 2510 and F9001440.

4.3.5 Space Requirements with Overlap Feature. – The overlap feature requires an additional block of approximately 15 K words of computer memory and will cause ORTEP to exceed the memory of a 32 K computer. For computers with a working storage under 45 K–60 K words, the overlap feature may be deleted by removing subroutines LAP500, LAP700, LAP800, LAPDRW, LAPAB, and LAPCON and substituting dummy subroutines for the first four of these six subroutines.

4.4 Addition of New OR TEP Instructions

Occasions will arise when additional special purpose instructions would be useful. For example, perhaps a cell outline routine would be desirable. (Originally, the 1000 series of instructions were planned for drawing a parallelepiped defined by four general vectors. However, this feature later seemed somewhat redundant and was omitted, since crystal cell outlines can be produced with judicious usage of small dummy atoms and the 800 series instructions.)

The subroutines F1000 and SPARE are intended to be used for additional instructions. All 1000 series instructions call subroutine F1000, which is currently just a dummy routine. Instructions $\geq$ 1200 call another dummy routine, subroutine SPARE(NJ), where NJ = instruction number/100.

All Arithmetic subprograms (see 4.2.3) and many of the subsidiary subprograms (see 4.2.2) are available for coding these Mainstream subprograms (see 4.2.1).

4.5 Glossary of Symbols in OR TEP Common, with Array Dimensions

	A(9)	Direct crystal cell parameters, a, b, c, cos α, cos β, cos γ, $\alpha(°)$, $\beta(°)$, $\gamma(°)$.
	AA(3,3)	Metric tensor **g** where $\mathbf{g}_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.
	AAREV(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the reference Cartesian system. **AAREV = AA REFV.**
	AAWRK(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the working Cartesian system. **AAWRK = AA WRKV.**
	AID(3,3)	Identity matrix.
	AIN(140)	Array containing the input parameters of the current OR TEP instruction.
	ATOMS(4,500)	Column 1 contains atom designator codes for the atoms which are to be included in the scaling, plotting, bond searching, etc. The other three columns are used for temporary storage of coordinates in any of several coordinate systems.
	BB(3,3)	Reciprocal metric tensor. **BB = AA**$^{-1}$.
P	BRDR	Border width in inches extending inward from plot boundary.
	CD(8,10)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(100)	Chemical symbols for the input atoms.
P	CONT(5)	Constants used in subroutine RADIAL.
	D(3,130)	Array in which three-dimensional points on an ellipse are stored by RADIAL.
	DA(3,3)	Transmits conjugate vectors to RADIAL. Also used for temporary storage.
	DP(2,130)	Array in which two-dimensional points for ellipse are stored after projection.
P	DISP	Displacement parameter for retracing.
	EDGE	Distance in inches from a projected point to the closest boundary. Set in PLTXY.
	EV(3,100)	Root-mean-square displacements for each principal axis of each input atom.
P	FORE	Cosine of critical angle between bond and Cartesian z axis vectors for perspective bond distance labels. At smaller angles the labels, produced from subroutine BOND, are drawn without perspective to prevent excessive foreshortening.
	FS(3,3,48)	Rotation matrices for input symmetry operations based on triclinic system. Used with TS array.
P	IN	Logical number for monitor input magnetic tape.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling ("Tilted Titles").
	KD(5,10)	Part of vector search code array. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
P	LTNO	Logical tape number for magnetic plotting tape.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction (vector search codes).

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	NG	FAULT INDICATOR (see 3.4).
	NJ	Instruction number/100.
	NJ2	Last two decimal digits of the instruction number (instruction = NJ*100 + NJ2).
P	NOUT	Logical number for monitor output magnetic tape.
P	NSR	Logical number for scratch magnetic tape.
	NSYM	Number of input symmetry operations.
P	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).
	P(3,100)	Triclinic positional coordinates for the input atoms.
	PA(3,3,100)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 A long, based on the triclinic system (principal axis vectors).
	PAC(3,5)	A 3 × 3 matrix produced by subroutine PAXES and made up of three orthonormal principal axis column vectors, based on either the working or reference Cartesian system. Columns 4 and 5 are used in subroutine F700 to duplicate columns 1 and 2 for ease in indexing.
	PAT(3,3)	A matrix produced by subroutine PAXES and composed of three principal axis column vectors each 1 A long, based on the triclinic system.
	Q(3,3)	A matrix produced by subroutine PAXES. Contains either the dispersion matrix or its inverse, based on either the working or reference Cartesian systems.
	REFV(3,3)	A matrix made up of three orthogonal column vectors, each 1 A long, based on the triclinic system. This is the base vector triplet for the reference Cartesian coordinate system. The transpose is the postfactor transformation matrix for converting coordinates from the reference orthogonal system to the triclinic system. $\mathbf{REFV}^T = \mathbf{AAREV}^{-1}$.
P	RES(4)	Regulates the resolution of the plotting of a given ellipse as a function of the longest principal axis x in the given ellipsoid of the scaled model.

$x \geqq$ Res(1)	128-point ellipse
Res(1) $> x \geqq$ Res(2)	64-point ellipse
Res(2) $> x \geqq$ Res(3)	32-point ellipse
Res(3) $> x$	16-point ellipse
Res(4) is not used.	

	RMS(5)	The rms displacements along the principal axes in arrays PAC and PAT.
P	SCAL1	The scale of the model in inches per angstrom before projection.
P	SCAL2	The scale factor ratio which sets the ellipsoid scale relative to SCAL1. If SCAL2 = 1.54, then the instantaneous position of the atomic center will be within the ellipsoid 50% of the time (50% probability ellipsoid).
P	SCL	SCL = SCAL1 times SCAL2.
P	SYMB(3,3)	A rotation matrix based on the angle THETA which is set by instruction 302.
P	TAPER	The exaggerated bond taper parameter. The top and bottom ends of a bond have radii: RADIUS = 1. ± TAPER *T6 where T6 = |cosine of angle between bond and z axis of Cartesian system| .

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	THETA	Angle in degrees between plotter x axis and lettering base-line vector.
	TITLE(12)	Alphanumeric job title storage.
	TITLE2(12)	Alphanumeric information storage for Format No. 3 trailer card.
	TS(3,48)	Translation vector for each input symmetry operation. Used with FS array.
P	VIEW	Viewing distance in inches.
	VT(3,4)	Perspective title rotation matrix and translation vector. Also used for temporary storage.
	V1(4)	Array to transfer data to subroutine STORE. Also used for temporary storage.
	V2(3) , ... , V6(3)	Temporary storage.
	WRKV(3,3)	Same definition as for REFV except that this one is for working Cartesian system. $\mathbf{WRKV}^T = \mathbf{AAWRK}^{-1}$.
P	XLNG(3)	Elements (1) and (2) are x and y plot dimensions. Element (3) is not used.
P	XO(3)	Elements (1) and (2) denote the position in plotter coordinates (in inches) where ORGN is placed. Element (3) is used to transfer Z coordinates to subroutine DRAW when perspective lettering is used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS

It is convenient to develop the physical significance of the anisotropic temperature factor with the notation and terminology of probability theory rather than with the more familiar Fourier transform theory. The results are, of course, identical regardless of the terminology used. The reason for this choice is that the literature of mathematical statistics and probability theory is somewhat neater and easier to follow. The texts by Wilks,[1] Cramer,[2] Miller,[3] Hamilton,[4] and Lukacs and Lana[5] and the handbooks by Burington and May[6] and Owen[7] are found to be particularly useful.

5.1 Probability Density Function (pdf) of a Trivariate Normal Distribution

Given three chance variables X_1, X_2, X_3 and S which is a region in X_1, X_2, X_3 space. The probability $P(S)$ that the point (X_1, X_2, X_3) falls in the region S is given by

$$P(S) = \iiint_S \phi(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 \,. \tag{5.1.1}$$

If the integration is carried over all space, then

$$\iiint_{-\infty}^{\infty} \phi(X_1, X_2, X_3)\, dX_1\, dX_2\, dX_3 = 1 \,. \tag{5.1.2}$$

The function $\phi(X_1, X_2, X_3)$ is called the probability density function (pdf) for the joint distribution of X_1, X_2, X_3. Using vector notation, we can designate the pdf as $\phi(\mathbf{X})$.

When the distribution is the type said to be normal or Gaussian, the pdf is

$$\phi(\mathbf{X}) = \frac{[\det(\mathbf{M}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp\left[-\tfrac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1}(\mathbf{X} - \hat{\mathbf{X}})\right] . \tag{5.1.3}$$

The matrix $\mathbf{M}^{-1}$ is the inverse of the symmetrical dispersion (variance-covariance) matrix $\mathbf{M}$, where

$$\mathbf{M} = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13} \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \sigma_2\sigma_3\rho_{23} \\ \sigma_1\sigma_3\rho_{13} & \sigma_2\sigma_3\rho_{23} & \sigma_3^2 \end{pmatrix} .$$

The symbols σ_i^2 represent the second moments or variances about the mean position $\hat{\mathbf{X}}$. The symbols $\sigma_i\sigma_j\rho_{ij}$ are the corresponding covariances and ρ_{ij} are the correlation coefficients.

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[1] S. S. Wilks, *Mathematical Statistics*, Wiley, New York, 1962.

[2] H. Cramer, *Random Variables and Probability Distributions*, Cambridge University Press, London, 1962.

[3] K. S. Miller, *Multidimensional Gaussian Distributions*, Wiley, New York, 1964.

[4] W. C. Hamilton, *Statistics in Physical Science*, Ronald, New York, 1964.

[5] E. Lukacs and R. G. Lana, *Applications of Characteristic Functions*, Hafner Publishing Co., New York, 1964.

[6] R. S. Burington and D. C. May, *Handbook of Probability and Statistics with Tables*, Handbook Publishers, Sandusky, Ohio, 1953.

[7] D. B. Owen, *Handbook of Statistical Tables*, Addison-Wesley, Reading, Mass., 1962.

5.2 Equiprobability Ellipsoids

For a proper normal distribution the quadratic form $(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1} (\mathbf{X} - \hat{\mathbf{X}})$ is positive definite, and a principal axis transformation is possible which will make the cross correlation coefficients $\rho_{ij} = 0$ $(i \neq j)$. This transformation is discussed in 5.4. The result of the transformation is the pdf

$$\phi(y_1, y_2, y_3) = \frac{1}{(2\pi)^{3/2} \sigma_{y_1} \sigma_{y_2} \sigma_{y_3}} e^{-Q/2} , \tag{5.2.1}$$

where

$$Q = \frac{(y_1 - \hat{y}_1)^2}{\sigma_{y_1}^2} + \frac{(y_2 - \hat{y}_2)^2}{\sigma_{y_2}^2} + \frac{(y_3 - \hat{y}_3)^2}{\sigma_{y_3}^2} . \tag{5.2.2}$$

The y_i are coordinates based on the Cartesian principal axis system and $\sigma_{y_i}^2$ are the variances along the principal axes, $i = 1, 2, 3$.

The normal probability density function is constant for points on the ellipsoid $Q = C^2$ where C is a constant. The probability that a random point (y_1, y_2, y_3) in the distribution will fall inside the ellipsoid is

$$P(C) = (2/\pi)^{1/2} \int_0^C r^2 e^{-r^2/2} \, dr . \tag{5.2.3}$$

This result is derived from (5.1.1), (5.2.1), and (5.2.2) by transforming to spherical coordinates.

When $C = 1.5382$, $P = 0.5$ and the corresponding ellipsoid is called the 50% probability ellipsoid. A table of P vs C values is found on page 203 of Owen's *Handbook of Statistical Tables.*[7] For convenience, that table is reproduced here as Table 5.1.

5.3 Characteristic Function (c.f.) of a Trivariate Normal Distribution

The characteristic function $\Phi(\mathbf{T})$ corresponding to a trivariate distribution $\phi(\mathbf{X})$ is the expected value of $e^{i\mathbf{T}^T\mathbf{X}}$, namely,

$$\Phi(\mathbf{T}) = \int_{-\infty}^{\infty} \phi(\mathbf{X}) e^{i\mathbf{T}^T\mathbf{X}} \, d\mathbf{X} . \tag{5.3.1}$$

For the trivariate normal pdf (5.1.3) the corresponding characteristic function is

$$\Phi(\mathbf{T}) = \exp\left[i\mathbf{T}^T\hat{\mathbf{X}} - \tfrac{1}{2}\mathbf{T}^T\mathbf{M}\mathbf{T}\right] , \tag{5.3.2}$$

where $\mathbf{M}$ is the variance-covariance dispersion matrix described in 5.1 and $\hat{\mathbf{X}}$ is the center of mass of the distribution.

The crystallographic structure factor equation which incorporates general anisotropic temperature factor coefficients is

$$F(\mathbf{h}) = \sum_n f_n(\mathbf{h}) \exp(2\pi i \mathbf{h}^T\hat{\mathbf{X}}_n) \exp(-\mathbf{h}^T\mathbf{B}_n\mathbf{h}) , \tag{5.3.3}$$

Table 5.1. Critical values for probability ellipsoids of a trivariate normal distribution[a]

P	C	P	C	P	C
0.01	0.3389	0.41	1.3842	0.81	2.1824
0.02	0.4299	0.42	1.4013	0.82	2.2114
0.03	0.4951	0.43	1.4183	0.83	2.2416
0.04	0.5479	0.44	1.4354	0.84	2.2730
0.05	0.5932	0.45	1.4524	0.85	2.3059
0.06	0.6334	0.46	1.4695	0.86	2.3404
0.07	0.6699	0.47	1.4866	0.87	2.3767
0.08	0.7035	0.48	1.5037	0.88	2.4153
0.09	0.7349	0.49	1.5209	0.89	2.4563
0.10	0.7644	0.50	1.5382	0.90	2.5003
0.11	0.7924	0.51	1.5555	0.91	2.5478
0.12	0.8192	0.52	1.5729	0.92	2.5997
0.13	0.8447	0.53	1.5904	0.93	2.6571
0.14	0.8694	0.54	1.6080	0.94	2.7216
0.15	0.8932	0.55	1.6257	0.95	2.7955
0.16	0.9162	0.56	1.6436	0.96	2.8829
0.17	0.9386	0.57	1.6616	0.97	2.9912
0.18	0.9605	0.58	1.6797	0.98	3.1365
0.19	0.9818	0.59	1.6980	0.99	3.3682
0.20	1.0026	0.60	1.7164	0.991	3.4019
0.21	1.0230	0.61	1.7351	0.992	3.4390
0.22	1.0430	0.62	1.7540	0.993	3.4806
0.23	1.0627	0.63	1.7730	0.994	3.5280
0.24	1.0821	0.64	1.7924	0.995	3.5830
0.25	1.1012	0.65	1.8119	0.996	3.6492
0.26	1.1200	0.66	1.8318	0.997	3.7325
0.27	1.1386	0.67	1.8519	0.998	3.8465
0.28	1.1570	0.68	1.8724	0.999	4.0331
0.29	1.1751	0.69	1.8932	0.9991	4.0607
0.30	1.1932	0.70	1.9144	0.9992	4.0912
0.31	1.2110	0.71	1.9360	0.9993	4.1256
0.32	1.2288	0.72	1.9580	0.9994	4.1648
0.33	1.2464	0.73	1.9804	0.9995	4.2107
0.34	1.2638	0.74	2.0034	0.9996	4.2661
0.35	1.2812	0.75	2.0269	0.9997	4.3365
0.36	1.2985	0.76	2.0510	0.9998	4.4335
0.37	1.3158	0.77	2.0757	0.9999	4.5943
0.38	1.3330	0.78	2.1012	0.99999	5.0894
0.39	1.3501	0.79	2.1274	0.999999	5.5376
0.40	1.3672	0.80	2.1544	0.9999999	5.9503

[a]Reproduced from Ref. 7 by permission of Addison-Wesley Publishing Company, Inc., Reading, Mass. The original caption was "Critical Values for the Spherical Normal Distribution."

where

$\mathbf{h}$ is a vector giving the Miller indices,

$\mathbf{X}_n$ is a vector giving the fractional unit cell coordinates of the nth atom,

$\mathbf{B}_n$ is the anisotropic temperature factor coefficient matrix, and

$f_n(\mathbf{h})$ is the atom form factor value for atom n.

If a change of variables $\mathbf{T} = 2\pi\mathbf{h}$ is made, then (5.3.3) can be rewritten as

$$F(\mathbf{T}) = \sum_n f_n(T) \exp\left(i\,\mathbf{T}^T\hat{\mathbf{X}}_n - \tfrac{1}{2}\,\mathbf{T}^T \frac{\mathbf{B}_n}{2\pi^2}\,\mathbf{T} \right) . \tag{5.3.4}$$

The scaled anisotropic temperature factor matrix $(1/2\pi^2)\mathbf{B}$ is seen to be identical with the variance-covariance dispersion matrix $\mathbf{M}$ in (5.3.2).

The corresponding crystal space trivariate normal pdf for any particular atom n is

$$\phi(\mathbf{X}) = \frac{[2\pi^2 \det(\mathbf{B}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp\left[-\pi^2(\mathbf{X} - \hat{\mathbf{X}})^T\mathbf{B}^{-1}(\mathbf{X} - \hat{\mathbf{X}})\right] ; \tag{5.3.5}$$

or if $\mathbf{M}^{-1} = 2\pi^2\mathbf{B}^{-1}$ then

$$\phi(\mathbf{X}) = \frac{\det(\mathbf{M}^{-1})}{(2\pi)^{3/2}} \exp\left[-\tfrac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T\mathbf{M}^{-1}(\mathbf{X} - \hat{\mathbf{X}})\right] , \tag{5.3.6}$$

which is identical to (5.1.3).

5.4 Principal Axis Transformation

The transformation of anisotropic temperature factor coefficients (for the general triclinic case) to principal axes of thermal motion is discussed by Waser,[8] Busing and Levy,[9] and Cruickshank *et al.*[10]

The principal axis transformation is necessary to find the thermal-motion probability ellipsoids discussed in 5.2. The principal axes of the matrix $\mathbf{M}^{-1}$ in (5.3.6) are the vectors $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ for which the inner vector product $(\mathbf{y}_i, \mathbf{y}_i)$ has a stationary value subject to the constraint

$$(\mathbf{y}_i, \mathbf{M}^{-1}\mathbf{y}_i) = 1 , \qquad i = 1, 2, 3 . \tag{5.4.1}$$

For the general triclinic crystal system this means that the quadratic form $\mathbf{y}^T\mathbf{G}^{-1}\mathbf{y}$ has a stationary value subjected to the constraint

$$\mathbf{y}^T\mathbf{G}^{-1}\mathbf{M}^{-1}\mathbf{y} = 1 , \tag{5.4.2}$$

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[8] J. Waser, *Acta Cryst.* **8**, 731 (1955).

[9] W. R. Busing and H. A. Levy, *Acta Cryst.* **11**, 450 (1958).

[10] D. W. J. Cruickshank *et al.*, p. 74 in *Computing Methods and the Phase Problem in X-Ray Crystal Analysis*, ed. by R. Pepinsky, J. M. Robertson, and J. C. Speakman, Pergamon, New York, 1961.

where $\mathbf{G}^{-1}$ is the metric tensor with components $\mathbf{a}_i \cdot \mathbf{a}_j$ and $\mathbf{a}_i \cdot \mathbf{a}_j$ is the scalar vector product of two of the three unit cell vectors. Introducing the Lagrange multiplier $1/\lambda$ leads to

$$\left[\mathbf{G}^{-1} - \frac{1}{\lambda_i}\mathbf{M}^{-1}\right]\mathbf{y}_i = 0 \qquad (i = 1,2,3); \tag{5.4.3}$$

premultiplying by $\mathbf{M}$ yields

$$\left[\mathbf{M}\mathbf{G}^{-1} - \frac{1}{\lambda_i}\mathbf{I}\right]\mathbf{y}_i = 0 \qquad (i = 1,2,3)\,. \tag{5.4.4}$$

Or we can do some additional rearranging and obtain

$$[\mathbf{G}\mathbf{M}^{-1} - \lambda_i\mathbf{I}]\,\mathbf{y}_i = 0 \qquad (i = 1,2,3)\,. \tag{5.4.5}$$

Equation (5.4.4) is equivalent to one of the results derived by Busing and Levy, except the λ_i obtained here are the reciprocals of their λ_i because we are doing the principal axis transformation on $\mathbf{M}^{-1}$ while their formulation performs the transformation on $\mathbf{M}$. The numerical procedure used in OR TEP finds the eigenvalues and eigenvectors of the unsymmetrical matrix $\mathbf{M}\mathbf{G}^{-1}$ in (5.4.4).

6. EXAMPLES OF ILLUSTRATIONS THAT HAVE BEEN PRODUCED WITH OR TEP

Most of the drawings reproduced here were made while OR TEP was under development. Consequently, certain details in the figures are not the same as those produced with the present version of the program. In particular, the lines of shading in the ellipsoid "open octant" are now always evenly spaced.

6.1 Nonstereoscopic Drawings Showing Thermal Motion

The figures in this section have the viewpoint at infinity (parallel projection).

6.1.1 Comparison of Graphical Representations of Thermal Motion. – Figure 6.1 shows the chelation pattern of two citrate molecules related by a twofold screw axis in the crystal structure of magnesium citrate decahydrate.[1] One molecule has "transparent ellipsoids" and the other has "opaque, plugged ellipsoids." Bond types 1, 3, and 4 (see 3.3.9) are illustrated. Note that certain bonds terminate at the ellipsoid boundary while others intersect the ellipsoid. These variables are under the user's control and can be used to advantage for special effects.

Figure 6.2 is another drawing of magnesium citrate decahydrate with the rms magnitudes of displacement along principal axes indicated around the equiprobability thermal ellipsoids.

Figure 6.3 illustrates the same figure with the thermal-motion representation mentioned by Waser,[2] in which the thermal motion is portrayed by a fourth-degree surface generated by a radius vector with length proportional to the rms component of displacement in the direction of the radius vector. The characteristic peanut shape of this fourth-degree surface is most apparent for atom O_3.

The thermal ellipsoid seems to be the preferred representation, and the present version of OR TEP will draw ellipsoids only.

6.1.2 Thermal Ellipsoids Derived from Independent Sets of Diffraction Data. – Figures 6.4(*a*) and (*b*) show the thermal ellipsoids for potassium dihydrogen isocitrate[3] obtained from two independent sets of three-dimensional x-ray data (copper K_α data and chromium K_α data). Figure 6.4(*a*) is presumably a better representation since it is based on a much larger number of measurements. In fact, it is rather surprising that the thermal-motion figures are so similar, considering the limited number of data obtainable with chromium radiation.

6.1.3 Thermal Motion in Molecules Not Related by Crystallographic Symmetry. – Myo-inositol[4] has two molecules in its crystallographic asymmetric unit. Figures 6.5(*a*) and 6.5(*b*) permit a comparison of the two sets of thermal ellipsoids in identical molecular orientations. The hydrogen bonds to neighboring atoms are also indicated. The similarity between the two ellipsoid sets is readily apparent.

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[1] C. K. Johnson, *Acta Cryst.*, 18, 1004 (1965) .

[2] J. Waser, *Acta Cryst.* **8**, 731 (1955).

[3] D. van der Helm, J. P. Glusker, C. K. Johnson, J. A. Minkin, N. E. Burow, and A. L. Patterson, *Acta Cryst.*, B-24, 578 (1968).

[4] I. N. Rabinowitz and J. Kraut, *Acta Cryst.* 17, 159 (1964).

6.2 Stereoscopic Drawings of Crystal Structures

6.2.1 Thermal Ellipsoids Derived from Neutron Studies. – Thermal ellipsoids for hydrogen atoms can be derived from neutron diffraction data. Some recent crystal structure results refined from three-dimensional neutron data are shown here as stereoscopic pairs of perspective projections. The thermal ellipsoid for a hydrogen atom is almost always larger than that of the heavier neighbor atom because of zero-point energy.

6.2.1.1 Chloral Hydrate. – Figure 6.6 features two molecules of chloral hydrate[5] related by a center of symmetry. The neighboring hydroxyl groups which are involved in hydrogen bonding to the two molecules are also included.

6.2.1.2 Sugars. – A single molecule of sucrose[6] is shown in Fig. 6.7 with the six-membered glucose ring to the left and the five-membered fructose ring to the right. Two intramolecular hydrogen bonds are drawn between the two moieties. Only one hydroxyl group in the molecule does not form a hydrogen bond; this group has the abnormally large thermal ellipsoid for hydrogen on the left side of the figure.

The thermal motion of a glucose molecule in the α-glucose crystal structure[7] is illustrated by Fig. 6.8. This figure was drawn with OR TEP by G. M. Brown.

6.2.1.3 Lithium Sulphate Monohydrate. – The inorganic structure lithium sulphate monohydrate has been refined with three-dimensional x-ray data by Larson[8] and with three zones of two-dimensional neutron data by Smith and Levy.[9] Figure 6.9 illustrates the characteristic atomic arrangement in that structure. The hydrogen thermal ellipsoids were taken from the neutron analysis and the remainder from the x-ray results. The outstanding feature in this illustration is the large thermal motion of the water molecule, which indicates much looser binding than in the rest of the structure.

6.2.1.4 Potassium Hydrogen Chloromaleate.[10] – This structure contains a centered hydrogen bond. The interatomic bond distances and the surrounding K atoms are also shown in Fig. 6.10, which was drawn with OR TEP by R. D. Ellison and H. A. Levy.

6.2.2 Thermal Ellipsoids Derived from X-Ray Studies. – The examples shown in this section were taken from the literature and from the work of several crystallographers who kindly sent their unpublished results to ORNL to be drawn.

6.2.2.1 Long-Chain Aliphatic Organic Compounds. – Dihydromalvalic acid[11] (cis, D, L-8,9-methylene-heptadecanoic acid) is shown in Fig. 6.11. The thermal motion perpendicular to the chain direction is seen to increase in amplitude toward the nonpolar end of the chain.

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[5] G. M. Brown and H. A. Levy, *Cryst. Struct. Commun.* **2**, 107 (1973).

[6] G. M. Brown and H. A. Levy, *Science* **141**, 921 (1963).

[7] G. M. Brown and H. A. Levy, *Science* **147**, 1038 (1965).

[8] A. C. Larson, *Acta Cryst.* **18**, 717 (1965).

[9] H. G. Smith, S. W. Peterson, and H. A. Levy, *J. Chem. Phys.* **48**, 5561 (1968).

[10] R. D. Ellison and H. A. Levy, *Acta Cryst.*, **19**, 260 (1965).

[11] G. A. Jeffrey and M. Sax, *Acta Cryst.* **16**, 1196 (1963).

Figure 6.12 illustrates the thermal motion in the triglyceride beta-tricaprin.[12] The two molecules shown are related by a center of symmetry. Again the amplitude of motion perpendicular to the chain increases toward the end of the chain.

6.2.2.2 Copper Chelation Compound. – The chelation pattern in *bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II)[13] is demonstrated in Fig. 6.13. The copper atom is on a symmetry center.

6.2.2.3 Large Biological Molecule. – Harunganin,[14] which is a plant pigment, is shown in Fig. 6.14. The pair of "half atoms" at the upper right is an approximation used in the least-squares refinement to correct for either very large thermal motion or disorder which occurs in that part of the crystal structure. The thermal parameters are somewhat questionable since the structure was not refined to convergence. However, the stereogram does permit the molecular configuration to be readily visualized.

6.2.2.4 Abnormal Motion in Cr(III) Acetylacetonate. – Dr. Bruno Morosin from Sandia Corporation sent this most unusual example of thermal motion. Cr(III) acetylacetonate[15] has three acetylacetonate ligands arranged to form an octahedral coordination of oxygens about the Cr atom, as shown in Fig. 6.15. One of the ligands displays very large thermal anisotropy. When a molecular packing diagram such as Fig. 6.16 is viewed, the large displacements are seen to be parallel to the **b** crystal axis. It appears that sheets of these ligands are either disordered or undergoing longitudinal vibration. Morosin has evidence from other diffraction experiments which supports the hypothesis that it is a thermal vibration phenomenon and not static disorder in the crystal.

6.2.3 Crystal Structure Packing Diagrams. – It is often desirable to illustrate the way that molecules pack together in a crystal structure. Sometimes thermal motion can be interpreted on this basis, as was done in 6.2.2.4. In other instances one may be more interested in visualizing the general packing geometry of the crystal structure. Stereograms are very useful for both applications.

6.2.3.1 Potassium Hydrogen Chloromaleate. – A molecule of this structure[10] is shown in Fig. 6.10. Packing diagrams were also drawn by Ellison and Levy and are reproduced here. Figure 6.17 shows the packing of anions about the two types of potassium ions. One coordination polyhedron is an irregular octahedron of oxygen atoms. The other is an irregular 14-hedron having six oxygen atoms and four chlorine atoms at its vertices. Figure 6.18 is a different view of the packing with a larger area included.

6.2.3.2 Packing Diagrams for Inorganic Structures. – The reader may have noticed that most of the illustrations are of organic structures. The reason is that organic molecules are easy to draw. Considerably more planning is required to produce an informative illustration of an inorganic structure.

An approach which is fairly successful is the following:

1. Draw a preliminary stereogram of the contents of a box which encloses somewhat more than one unit cell. Bonds should be drawn in accordance with known interatomic distance ranges. The dimensions

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[12] A. J. Mabis and L. H. Jensen, *Abstracts ACA Meeting, Bozeman, Montana*, F-9 (1964) and L. H. Jensen, private communication, 1964.

[13] G. E. Gurr, *Acta Cryst.* B24, 1511 (1968) and private communication, 1964.

[14] R. A. Alden, G. H. Stout, J. Kraut, and D. F. High, *Acta Cryst.* 17, 109 (1964).

[15] B. Morosin, *Acta Cryst.* 19, 131 (1965) and B. Morosin, private communication, 1964.

for this drawing may be such that the plot can be viewed directly with a stereoscope without photographic reduction.

2. While viewing the preliminary stereogram, pick out the basic structural units and decide on a grouping of these units for the desired figure.

3. Describe the intended subject with whichever technique is the most convenient and draw the new figure. Figure 6.19, potassium perxenate nonahydrate,[16] is an example of an illustration planned in this way. This figure was drawn by J. H. Burns at ORNL.

6.2.3.3 Illustrations of the Contents of a Unit Cell. – A favorite method used by crystallographers is to draw a unit cell outline and the cell contents within that outline. Figure 6.20, which is a stereogram showing lithium α-monodeuteroglycolate,[17] is of this nature. The molecules were kept intact rather than cut off at the cell outline.

6.3 Helical Structures

OR TEP has certain features which facilitate the drawing of nonintegral helical screw models such as those discussed in the field of molecular biology. The Pauling, Corey, and Branson alpha-helix model[18] for protein structure is an example. Figure 6.21 shows the modification of this structure which is present in the synthetic polypeptide poly-L-alanine.[19]

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[16] A. Zalkin, J. D. Forrester, D. H. Templeton, S. M. Williamson, and C. W. Koch, *J. Am. Chem. Soc.* **86**, 3569 (1964).

[17] C. K. Johnson, E. J. Gabe, M. R. Taylor, and I. A. Rose, *J. Am. Chem. Soc.* **87**, 1802 (1965).

[18] L. Pauling, R. B. Corey, and H. R. Branson, *Proc. Natl. Acad. Sci. U.S.* **37**, 235 (1951).

[19] A. Elliott and B. R. Malcolm, *Proc. Roy. Soc. London* **A 249**, 30 (1959).

ORNL DWG. 65-2448

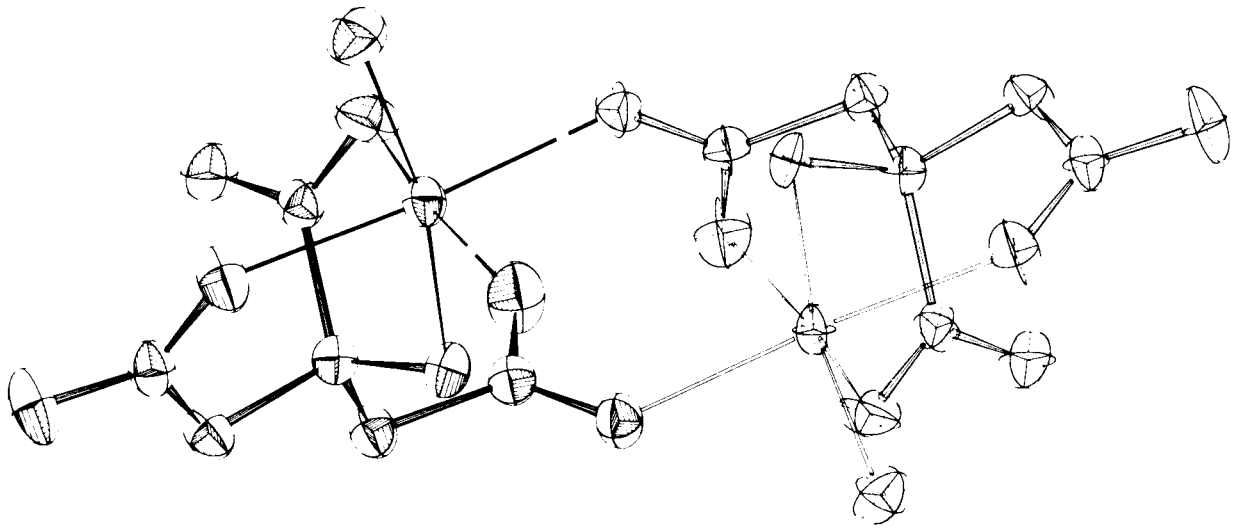

Fig. 6.1. Chelation Pattern Viewed Along a Twofold Screw Axis in the Crystal Structure of Magnesium Citrate Decahydrate. Ellipsoids represent equiprobability surfaces of thermal displacement and contain 65% of the probability distribution.

ORNL DWG. 65-2443

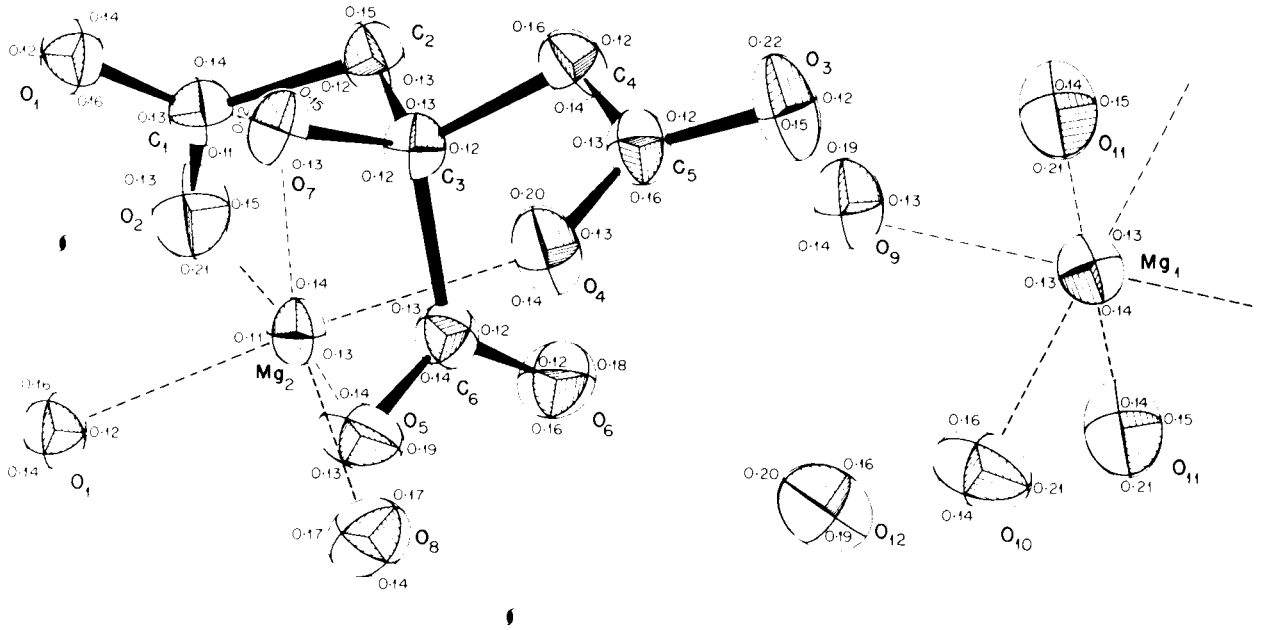

Fig. 6.2. Thermal-Ellipsoid Representation for Magnesium Citrate Decahydrate with Principal Values of RMS Displacement in Angstrom Units. Ellipsoids enclose 74% probability. Structure is viewed along *b* axis.

ORNL DWG. 65-2444

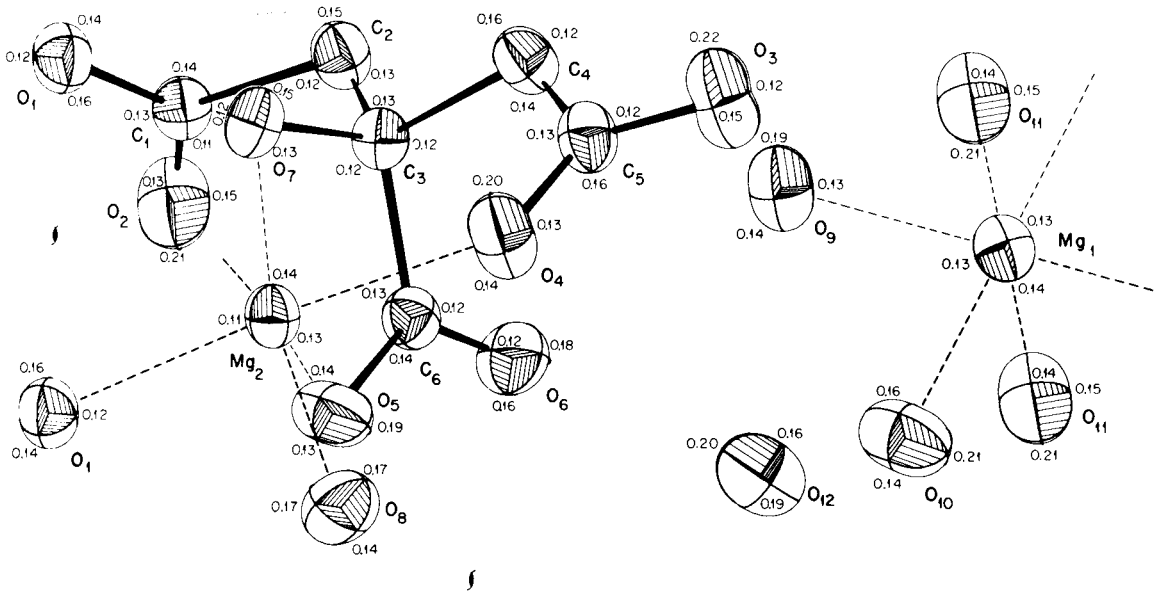

Fig. 6.3. Peanut-Shaped RMS Thermal-Displacement Figure Representation for Magnesium Citrate Decahydrate. Principal values of rms displacement in Angstrom units are indicated around the displacement figures, which are drawn at double scale. Same view of structure as shown in Fig. 6.2.

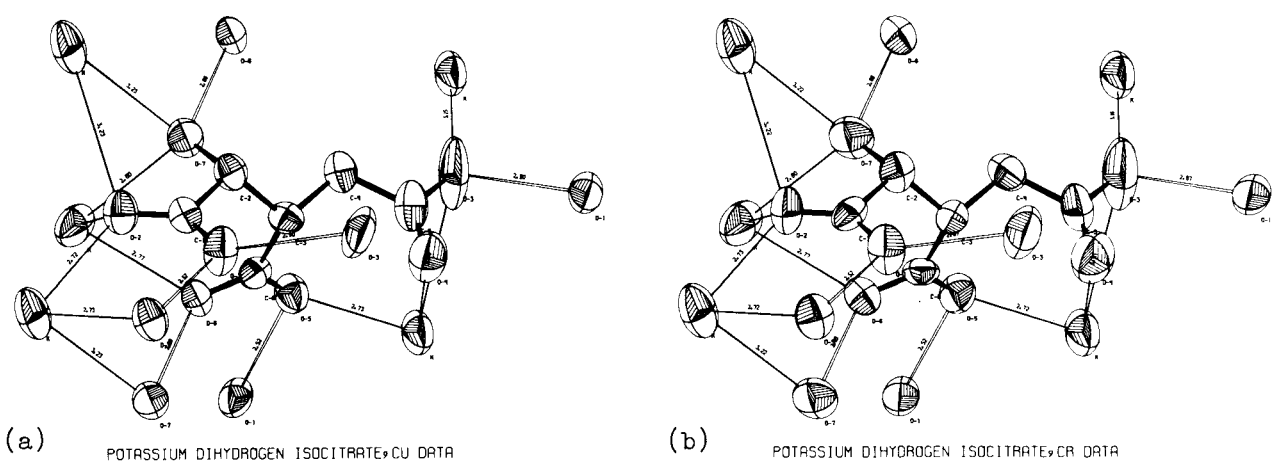

Fig. 6.4. Potassium Dihydrogen Isocitrate with Thermal Ellipsoids Scaled to Include 74% Probability. (*a*) Results obtained from 1350 three-dimensional copper K_α data (disagreement factor 6.5%). (*b*) Results obtained from 340 three-dimensional chromium K_α data (disagreement factor 2.2%). Note: This is *not* a stereo pair.

ORNL DWG. 65-2450

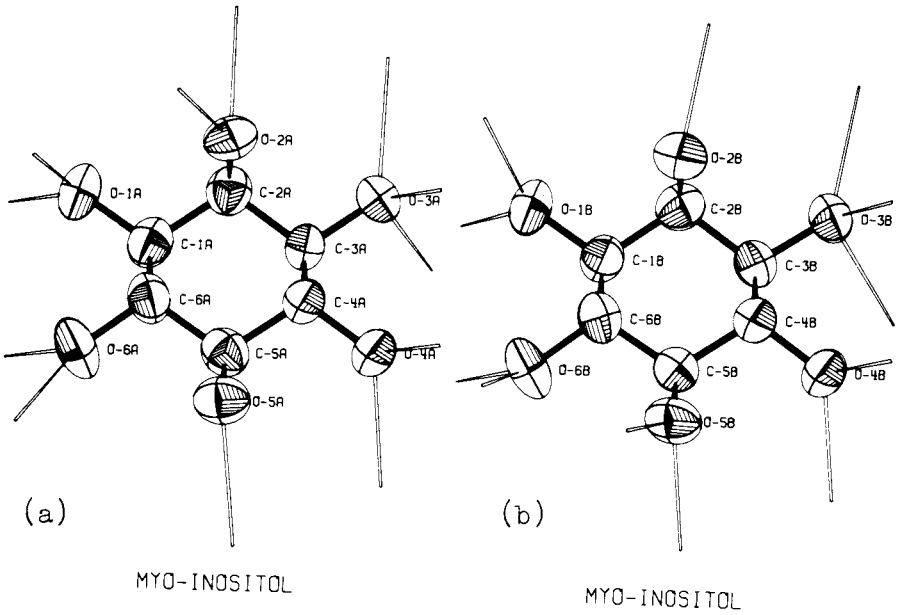

Fig. 6.5. Comparison of Thermal Ellipsoids in the Two Crystallographically Independent Molecules of Myo-Inositol (6.5*a* and 6.5*b*). Hydrogen bonding is shown, since this might influence the thermal motion. Ellipsoids are scaled to include 74% probability. Note: This is *not* a stereo pair.

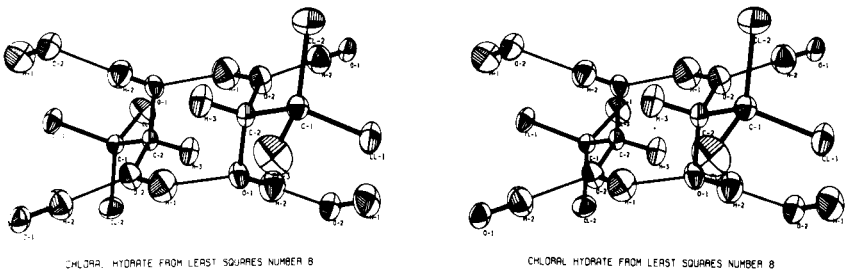

Fig. 6.6. Stereogram (Stereoscopic Pair of Perspective Projections) of Chloral Hydrate Viewed Along the Reciprocal Axis a^*. Two molecules are shown related by a center of symmetry, with the hydrogen bonds connecting them together and to other molecules. Ellipsoids are scaled to include 48% probability.

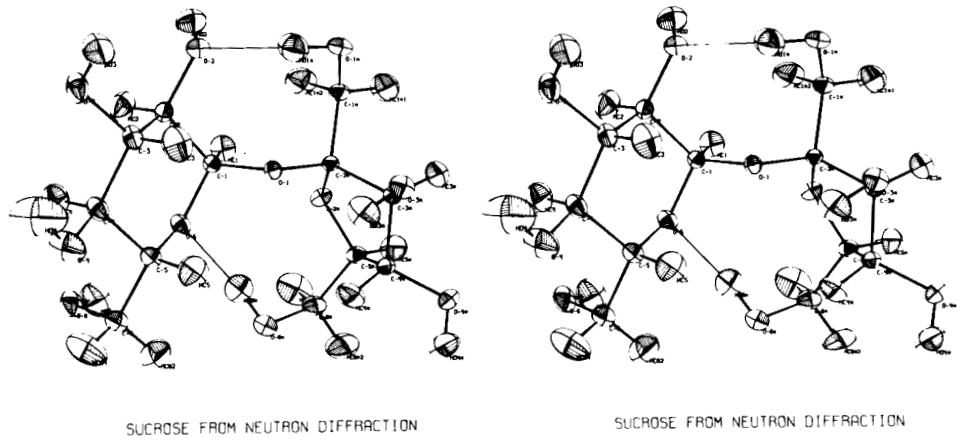

Fig. 6.7. Stereogram Showing the Sucrose Molecule with Thermal Ellipsoids Scaled to Enclose 50% Probability.

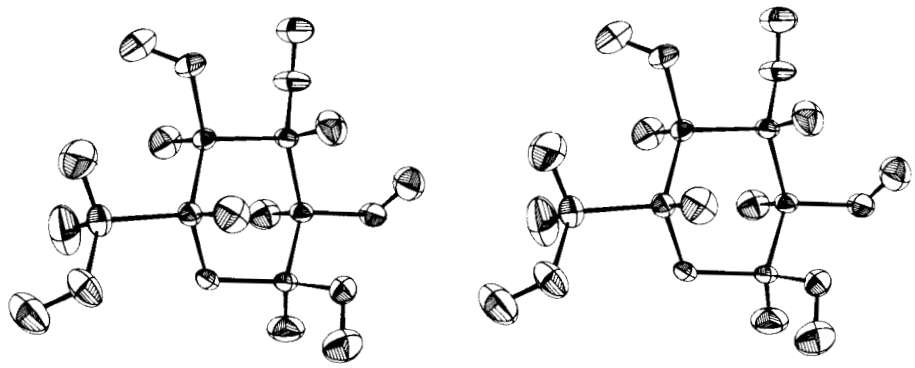

Fig. 6.8. A Molecule of Glucose with Thermal Ellipsoids Scaled to Enclose 50% Probability.

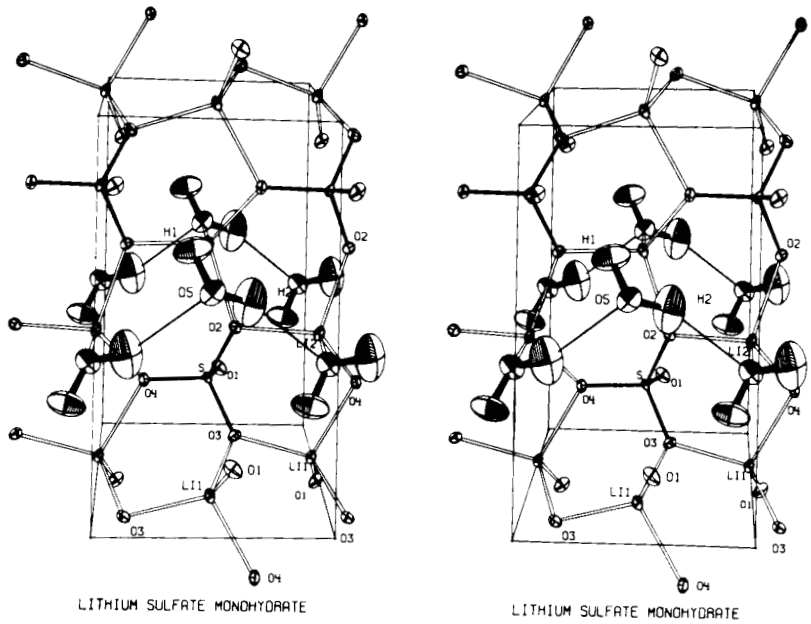

Fig. 6.9. Lithium Sulphate Monohydrate. The lithium ions and sulphate ions are coordinated into a compact network. The structure is viewed along the reciprocal a^* axis. The ellipsoids are scaled to enclose 20% probability.

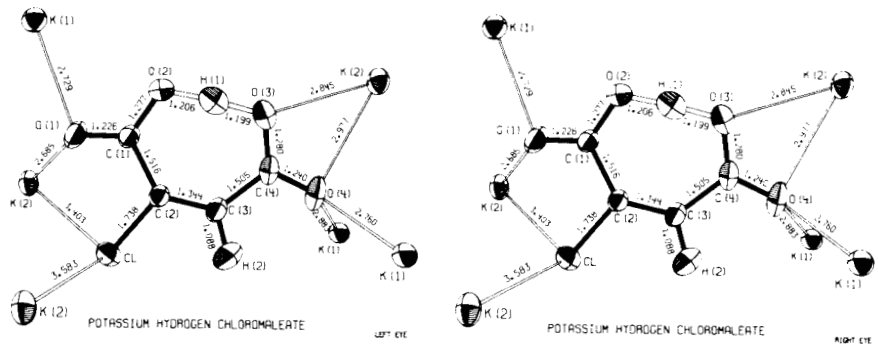

Fig. 6.10. Potassium Hydrogen Chloromaleate. The chloromaleate ion is viewed normal to its own plane. The thermal ellipsoids enclose 50% probability.

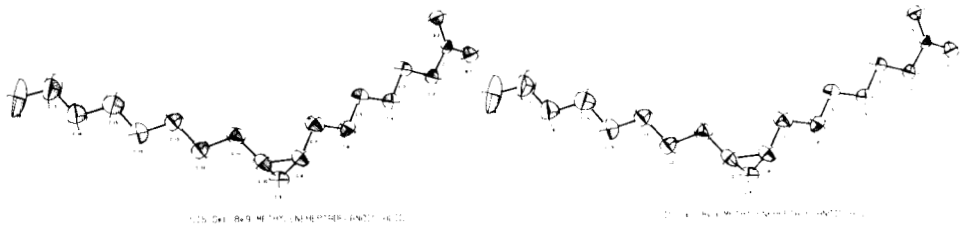

Fig. 6.11. A Molecule of Dihydromalvalic Acid with Thermal Ellipsoids Scaled to Enclose 48% Probability.

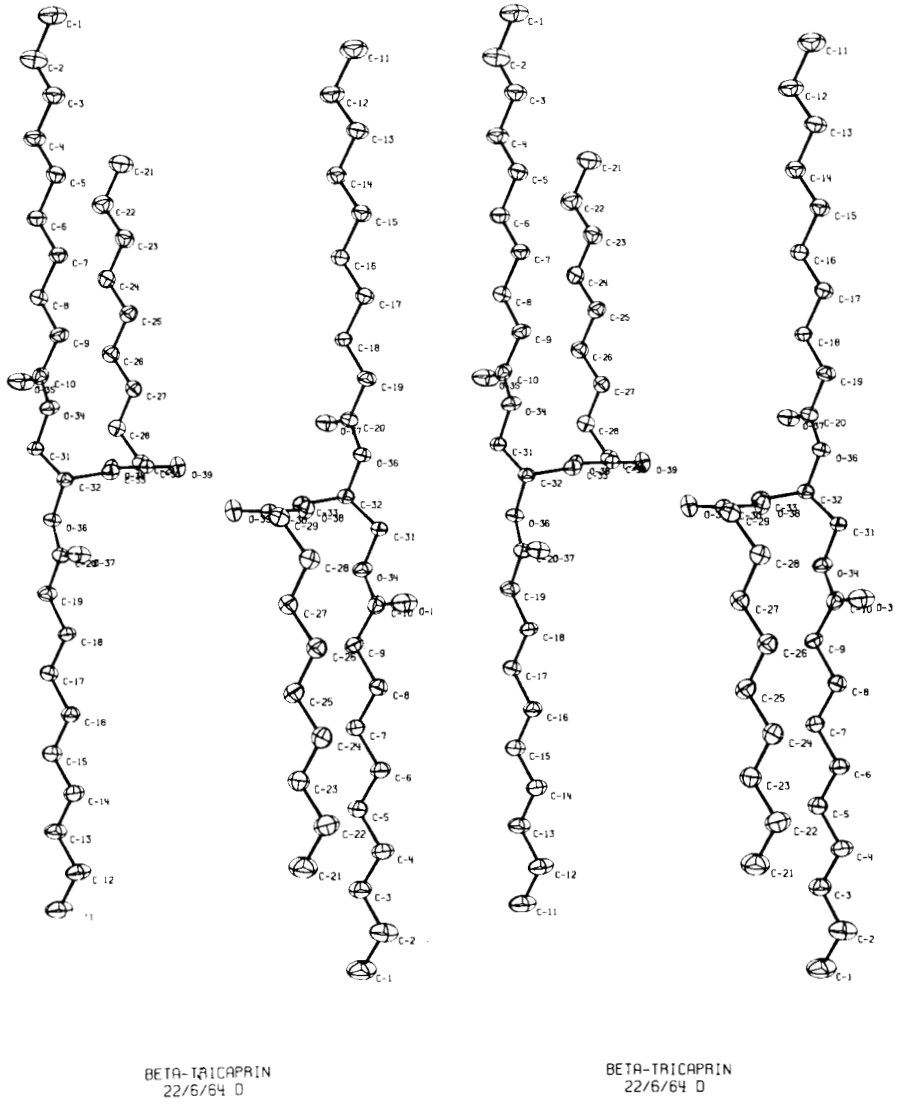

Fig. 6.12. Two Molecules of Beta-Tricaprin Related by a Center of Symmetry. The thermal ellipsoids are scaled to include 30% probability.

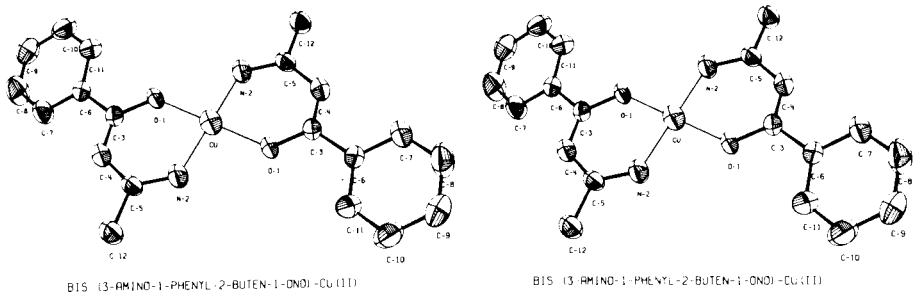

Fig. 6.13. Chelation Complex of *Bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

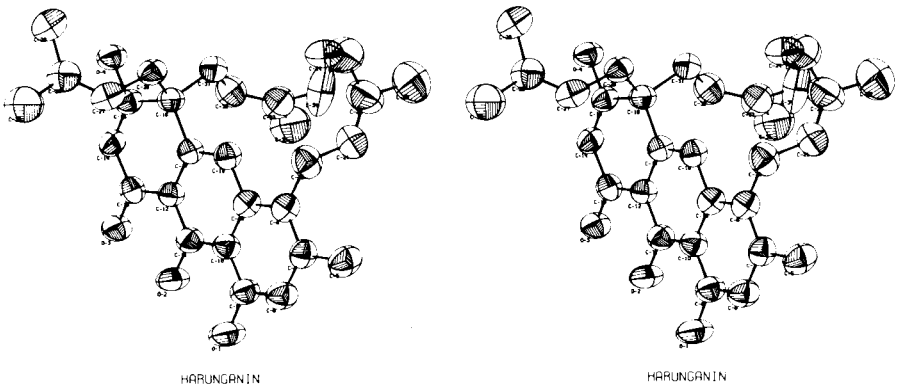

Fig. 6.14. A Molecule of the Plant Pigment Harunganin with Thermal Ellipsoids Scaled to Include 48% Probability.

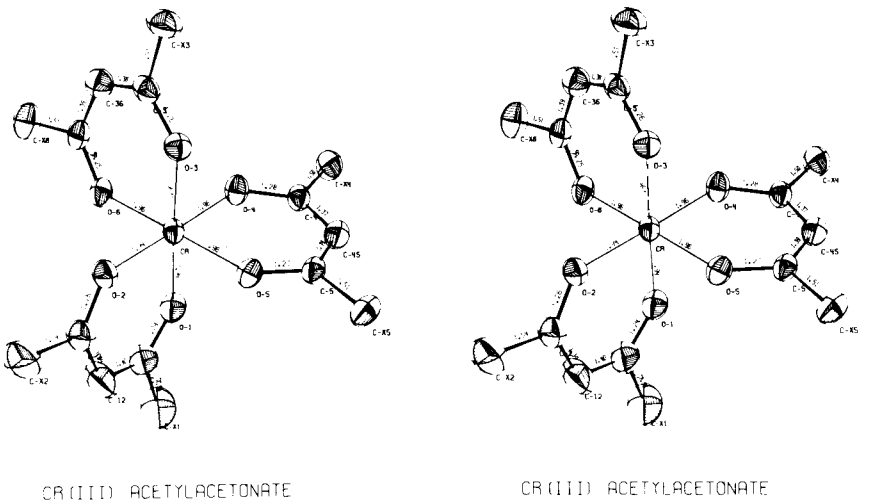

Fig. 6.15. A Unit of *Tris*-acetylacetonatochromium(III) Viewed Along its Threefold Axis of Chemical Symmetry. The thermal ellipsoids are scaled to enclose 20% probability.

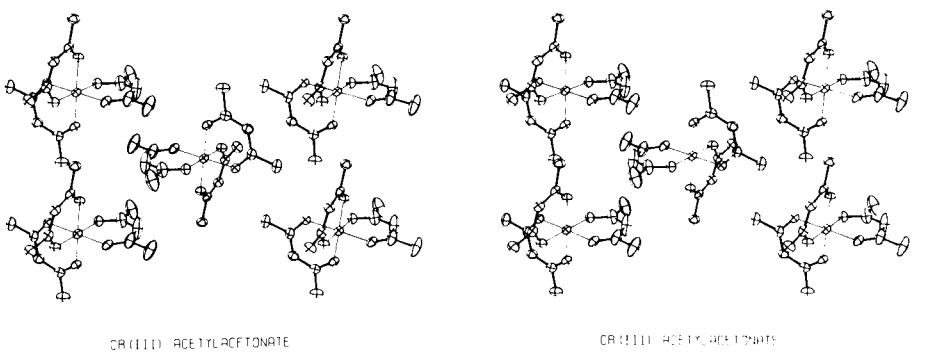

Fig. 6.16. Packing Diagrams for *Tris*-acetylacetonatochromium(III) Viewed Along the Reciprocal Axis c*. Thermal ellipsoids are scaled to enclose 20% probability.

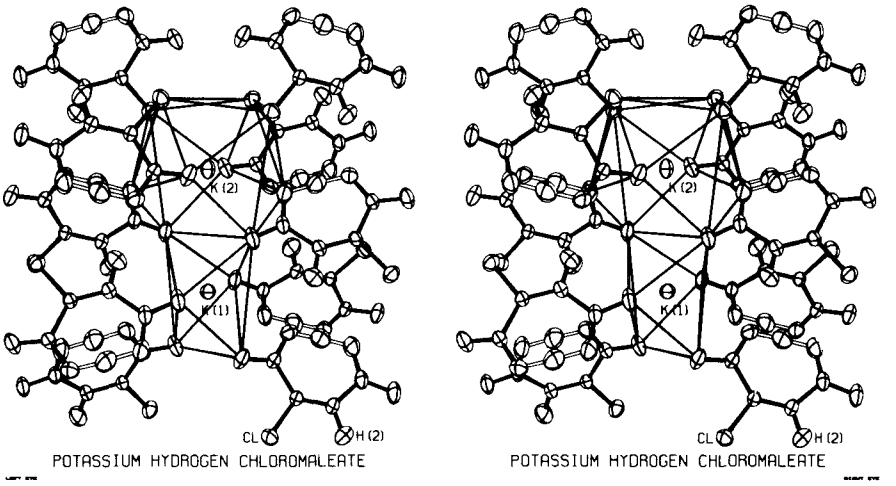

Fig. 6.17. Packing of Chloromaleate Ions Around the Potassium Ions in Potassium Hydrogen Chloromaleate. The edges of the coordination polyhedra are shown. View is nearly along the *c* axis. Thermal ellipsoids are scaled to contain 50% probability.

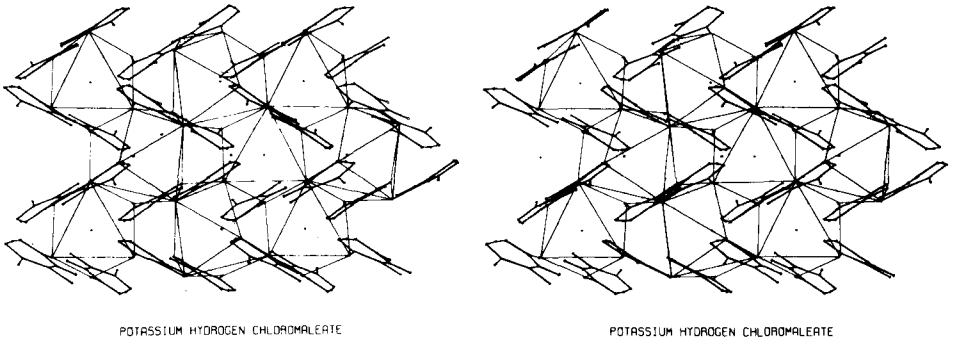

Fig. 6.18. Packing Diagrams for Potassium Hydrogen Chloromaleate. Atoms are represented as small circles. The edges of the coordination polyhedra around the potassium ions are shown. View is nearly along the *a* axis.

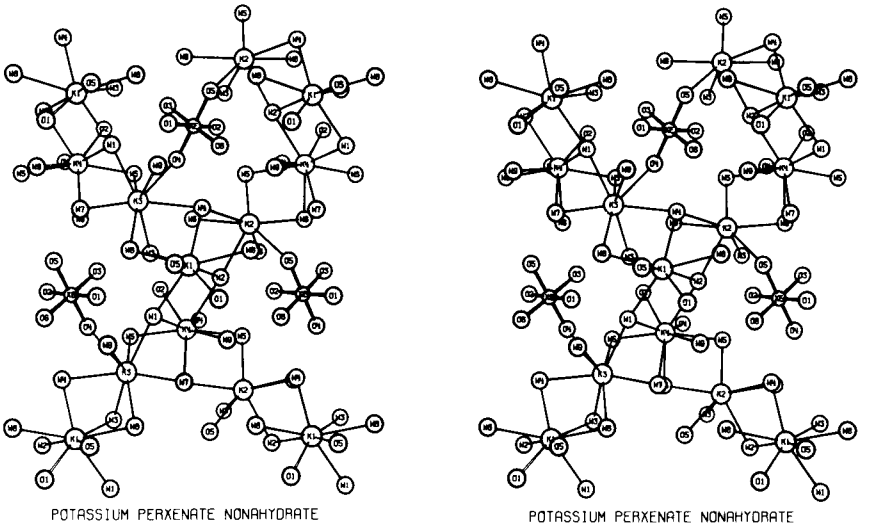

Fig. 6.19. Packing Diagram for Potassium Perxenate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Perxenate Ions. The view is parallel to the *a* axis. Another layer, related to the present one by a twofold screw axis along *a*, is needed to complete the structure.

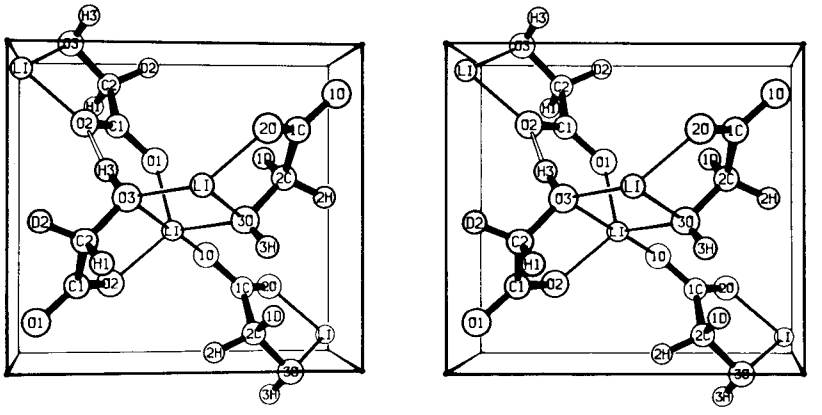

Fig. 6.20. A Stereogram Showing the Unit-Cell Contents of Anhydrous Li α-monodeuteroglycolate. The unique monoclinic *b* axis points up in the page and the mean *c* axis out from the page.

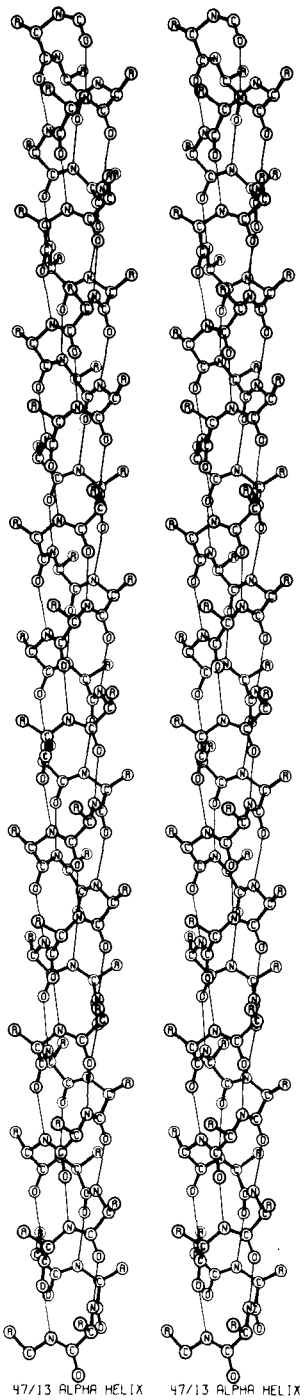

Fig. 6.21. A Stereoscopic Pair of Perspective Projections Showing the Alpha-Helix Which Is Present in Poly-L-Alanine. There are 47 amino-acid residues in 13 turns of the helix. Stereo viewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP-II

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C     TOTAL NUMBER OF CARDS INCLUDING DATA FOR EXAMPLE IS 4745          MAIN  10
C     ***** OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM ****               MAIN  20
C     ***** ORTEP-II / IBM-360 / FEB 1971 / INSTRUCTIONS IN CRNL-3794 **MAIN  30
C     ***** OPTIONAL OVERLAP FEATURE ADDED TO ORTEP IN FEBRUARY 1971 ***MAIN  40
C     ***** CUBANE EXAMPLE CARDS ILLUSTRATE USE OF OVERLAP FEATURE *****MAIN  50
C     ***** IN BRIEF, INSTRUCTION 511 MAY BE USED JUST BEFORE EACH      MAIN  60
C     ***** DRAWING TO STORE THE PROJECTED ATOMS, TYPE 2 TRAILER CARDS  MAIN  70
C     ***** WITH INSTR 511 CAUSES PROJECTED BONDS ALSO TO BE STORED     MAIN  80
C     ***** MAXIMUM NUMBER OF STORED BONDS IS 599.  IN GENERAL, JUST USEMAIN  90
C     ***** THE SAME TYPE 2 TRAILER CARDS USED BY THE 802/812 INSTR. ***MAIN 100
C     ***** COLS 10-18 ON 511 INST CARD SPECIFIES OVERLAP MARGIN(OVMRGN)MAIN 110
C     *****          0       OVMRGN = MAX(0.035 OR SQRT(SCAL1)*0.030)   MAIN 120
C     *****      1 OR -1     OVMRGN = 0.0                               MAIN 130
C     *****    .GT.0,.LT.1  OVMRGN = ACTUAL VALUE GIVEN (INCHES) *****  MAIN 140
C     ***** ALL OVERLAP INFORMATION IS DESTROYED BY INSTR. 501-510      MAIN 150
C     ***** IF THE COMPUTER MEMORY AVAILABLE IS EXCEEDED BY THIS FEATUREMAIN 160
C     ***** SUBROUTINES LAP500, LAP700, LAP800, LAPDRW, LAPAB AND LAPCONMAIN 170
C     ***** MAY BE REMOVED AND REPLACED BY THE FOLLOWING 4 DUMMIES      MAIN 180
C     SUBROUTINE LAP500(NTYPE)                                          MAIN 190
C     RETURN                                                            MAIN 200
C     END                                                               MAIN 210
C     SUBROUTINE LAP700(NA,ICQ)                                         MAIN 220
C     RETURN                                                            MAIN 230
C     END                                                               MAIN 240
C     SUBROUTINE LAP800(NA1,NA2,ICQ)                                    MAIN 250
C     RETURN                                                            MAIN 260
C     END                                                               MAIN 270
C     SUBROUTINE LAPDRW(Y,NPEN,NCQ)                                     MAIN 280
C     RETURN                                                            MAIN 290
C     END                                                               MAIN 300
      REAL*8 CHEM                                                       MAIN 310
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    MAIN 320
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)MAIN 330
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) MAIN 340
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) MAIN 350
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   MAIN 360
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   MAIN 370
      DIMENSION XLNG(3),XO(3),XT(3)                                     MAIN 380
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   MAIN 390
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD MAIN 400
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1MAIN 410
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   MAIN 420
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                MAIN 430
      LTNO=0                                                            MAIN 440
    2 CALL PRIME                                                        MAIN 450
C     ***** READ JOB TITLE CARD *****                                   MAIN 460
      READ (IN,4)(TITLE(I),I=1,18)                                      MAIN 470
    4 FORMAT(18A4)                                                      MAIN 480
      WRITE (NOUT,6)(TITLE(I),I=1,18)                                   MAIN 490
    5 FORMAT(1H010X,18A4)                                               MAIN 500
    6 FORMAT(1H110X,18A4)                                               MAIN 510
      CALL PRELIM                                                       MAIN 520
      WRITE (NOUT,6)(TITLE(I),I=1,18)                                   MAIN 530
      ISAVE=0                                                           MAIN 540
      GO TO 507                                                         MAIN 550
    7 ISAVE=0                                                           MAIN 560
C     ***** ZERO AIN ARRAY *****                                        MAIN 570
    8 DO 10 J=1,140                                                     MAIN 580
   10 AIN(J)=0.                                                         MAIN 590
   11 FORMAT(1H04X,17H(((((INSTRUCTIONI5,6H )))))                       MAIN 600
   12 FORMAT(I3,I6,7F9.0)                                               MAIN 610
   13 FORMAT(I3,I6,7E15.8)                                              MAIN 620
   14 FORMAT(1H 9X,7E15.7)                                              MAIN 630
C     ***** READ NEW INSTRUCTION CARD *****                             MAIN 640
      NCD=0                                                             MAIN 650
      N1=-6                                                             MAIN 660
   16 N1=N1+7                                                           MAIN 670
      N2=N1+6                                                           MAIN 680
      IF(ISAVE)22,18,18                                                 MAIN 690
   18 READ (IN,12)IC,NF,(AIN(I),I=N1,N2)                                MAIN 700
      IF(ISAVE)24,24,20                                                 MAIN 710
   20 WRITE (NSR)IC,NF,(AIN(I),I=N1,N2)                                 MAIN 720
      GO TO 24                                                          MAIN 730
   22 READ (NSR)IC,NF,(AIN(I),I=N1,N2)                                  MAIN 740
      IF(IC)7,24,24                                                     MAIN 750
   24 IF(N1-1)26,26,30                                                  MAIN 760
   26 WRITE (NOUT,11)NF                                                 MAIN 770
      NF1=NF                                                            MAIN 780
      IF(NF1)28,8,30                                                    MAIN 790
   28 IF(NF1+2)2,2,3000                                                 MAIN 800
   30 WRITE (NOUT,14)(AIN(I),I=N1,N2)                                   MAIN 810
   32 IC=IC+1                                                           MAIN 820
      GO TO (90,16,38,50),IC                                            MAIN 830
   33 FORMAT(I3,6X,5I3,8F6.0)                                           MAIN 840
   34 FORMAT(6I3,8E12.5)                                                MAIN 850
   35 FORMAT(1H 11X,5I3,8F11.5)                                         MAIN 860
C     ***** READ FORMAT 2 TRAILER CARDS *****                           MAIN 870
   38 NCD=NCD+1                                                         MAIN 880
      IF(ISAVE)44,40,40                                                 MAIN 890
   40 READ (IN,33)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                MAIN 900
      IF(ISAVE)46,46,42                                                 MAIN 910
   42 WRITE (NSR)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                 MAIN 920
      GO TO 46                                                          MAIN 930
   44 READ (NSR)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                  MAIN 940
   46 WRITE (NOUT,35)(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                MAIN 950
      GO TO 32                                                          MAIN 960
C     ***** READ FORMAT 3 TRAILER CARD *****                            MAIN 970
   50 IF(ISAVE)52,54,54                                                 MAIN 980
   52 READ (NSR)(TITLE2(I),I=1,18)                                      MAIN 990
      GO TO 55                                                          MAIN1000
   54 READ (IN ,4)(TITLE2(I),I=1,18)                                    MAIN1010
   55 WRITE (NOUT,5)(TITLE2(I),I=1,18)                                  MAIN1020
      IF(ISAVE)90,90,56                                                 MAIN1030
   56 WRITE (NSR)(TITLE2(I),I=1,18)                                     MAIN1040
C     ***** EXECUTE INSTRUCTION *****                                   MAIN1050
   90 NJ=NF1/100                                                        MAIN1060
      NJ2=NF1-NJ*100                                                    MAIN1070
      NJ3=MOD(NJ2,10)                                                   MAIN1080
      IF(NJ-12)98,92,92                                                 MAIN1090
   92 CALL SPACE(NF1)                                                   MAIN1100
      IF(NG)94,8,94                                                     MAIN1110
   94 CALL ERPNT(0.,NF1)                                                MAIN1120
      GO TO 8                                                           MAIN1130
C     ******BRANCH TABLE FOR FUNCTION TYPES******                       MAIN1140
   98 GO TO(100,200,300,400,500,600,700,800,900,1000,1100),NJ           MAIN1150
C     *******STRUCTURE ANALYSIS FUNCTIONS*******                        MAIN1160
  100 GO TO (101,101,104,104,101,101,94),NJ2                            MAIN1170
  101 CALL SEARC                                                        MAIN1180
      GO TO 8                                                           MAIN1190
C     ***** ANISOTROPIC TEMP FACTOR OUTPUT *****                        MAIN1200
  104 DO 164 I=1,NATOM                                                  MAIN1210
      IF(MOD(I,14)-1)134,114,134                                        MAIN1220
  114 WRITE (NOUT,6)(TITLE(J),J=1,18)                                   MAIN1230
      WRITE (NOUT,129)                                                  MAIN1240
  129 FORMAT(1H010X,4HATOM3X,16HRMS DISPLACEMENT3X,31HROW VECTORS, BASEDMAIN1250
     1 ON REFERENCE17X,29HPROBABILITY COVARIANCE MATRIX)                MAIN1260
  134 T1=55501.+FLOAT(I)*100000.                                        MAIN1270
      CALL PAXES(T1,-3)                                                 MAIN1280
      IF(NG)144,154,144                                                 MAIN1290
  144 CALL ERPNT(T1,104)                                                MAIN1300
  149 FORMAT(1H010X,A6,F10.6,6X,3F12.7,10X,3F12.7)                      MAIN1310
  154 WRITE (NOUT,149)CHEM(I),RMS(1),(PAC(J,1),J=1,3),(Q(J,1)           MAIN1320
     1,J=1,3)                                                           MAIN1330
  164 WRITE (NOUT,159)(RMS(K),(PAC(J,K),J=1,3),(Q(J,K),J=1,3)           MAIN1340
     1,K=2,3)                                                           MAIN1350
  159 FORMAT(1H 16X,F10.6,6X,3F12.7,10X,3F12.7)                         MAIN1360
      GO TO 8                                                           MAIN1370
C     *******PLOTTER INITIALIZE,FRAME ADVANCE,TERMINATE FUNCTIONS*******MAIN1380
  200 CALL F200                                                         MAIN1390
      GO TO 8                                                           MAIN1400
  300 GO TO (301,302,303,94),NJ2                                        MAIN1410
C     *******PLOT DIMENSIONS*******                                     MAIN1420
  301 IF(AIN(1))321,321,311                                             MAIN1430
  311 XLNG(1)=AIN(1)                                                    MAIN1440
  321 IF(AIN(2))341,341,331                                             MAIN1450
  331 XLNG(2)=AIN(2)                                                    MAIN1460
  341 IF(AIN(3))361,351,351                                             MAIN1470
  351 VIEW=AIN(3)                                                       MAIN1480
  361 IF(AIN(4))381,381,371                                             MAIN1490
  371 BRDR=AIN(4)                                                       MAIN1500
  381 WRITE (NOUT,389)XLNG(1),XLNG(2),BRDR                              MAIN1510
  389 FORMAT(1H010X,11HPLOT LIMITSF6.2,3H BYF6.2,15H IN.  INCLUDINGF6.2,MAIN1520
     112H  IN. MARGIN)                                                  MAIN1530
  391 WRITE (NOUT,399)VIEW                                              MAIN1540
  399 FORMAT(1H 10X,13HVIEW DISTANCEF7.3,7H INCHES)                     MAIN1550
      GO TO 8                                                           MAIN1560
C     *******LEGEND ROTATION*******                                     MAIN1570
  302 THETA=AIN(1)                                                      MAIN1580
      T1=THETA*.01745329252                                             MAIN1590
      COSTH=COS(T1)                                                     MAIN1600
      SINTH=SIN(T1)                                                     MAIN1610
      DO 312 J=1,9                                                      MAIN1620
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  312 SYMB(J,1)=0.
      SYMB(1,1)=COSTH                                                   MAIN1630
      SYMB(2,2)=COSTH                                                   MAIN1640
      SYMB(3,3)=1.                                                      MAIN1650
      SYMB(2,1)=SINTH                                                   MAIN1660
      SYMB(1,2)=-SINTH                                                  MAIN1670
      WRITE (NOUT,319)THETA                                             MAIN1680
  319 FORMAT(1H010X,44HREGULAR TITLE AND SYMBOL ROTATION IN DEGREESF8.2) MAIN1690
      GO TO 8                                                           MAIN1700
C     ***** RETRACE DISPLACEMENT *****                                  MAIN1710
  303 DISP=AIN(1)                                                       MAIN1720
      WRITE (NOUT,313)DISP                                              MAIN1730
  313 FORMAT(1H010X,22HRETRACE DISPLACEMENT =F7.4,5H INCH)              MAIN1740
      GO TO 8                                                           MAIN1750
C     *******ATOM LIST FUNCTIONS*******                                 MAIN1760
  400 GO TO (401,401,401,401,401,401,490, 94, 94,410,                   MAIN1770
     1       401,401,401,401,401,401, 94),NJ2                           MAIN1780
  401 CALL F400                                                         MAIN1790
      GO TO 490                                                         MAIN1800
  410 LATM=0                                                            MAIN1810
      DO 420 I=1,500                                                    MAIN1820
      DO 420 J=1,4                                                      MAIN1830
  420 ATOMS(J,I)=0.                                                     MAIN1840
  490 IF(LATM)8,8,491                                                   MAIN1850
  491 WRITE (NOUT,499)(ATOMS(1,I),I=1,LATM)                             MAIN1860
  499 FORMAT(1H010X,23HCONTENTS OF ATOMS ABRAY/(15X,10F10.0))           MAIN1870
      GO TO 8                                                           MAIN1880
C     *******CARTESIAN COORDINATE SYSTEM FUNCTIONS*******               MAIN1890
  500 CALL F500                                                         MAIN1900
      WRITE  (NOUT,503)(ORGN(J),J=1,3)                                  MAIN1910
  503 FORMAT(1H0,10X,     44HORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.MAIN1930
     1,3F15.6)                                                          MAIN1940
      IF(NJ3-3)507,539,504                                              MAIN1950
  504 IF(NJ3-6)601,507,601                                              MAIN1955
  507 WRITE (NOUT,529)                                                  MAIN1960
      WRITE (NOUT,519)((REFV(J,I),I=1,3),(AAREV(J,I),I=1,3),J           MAIN1970
     1=1,3)                                                             MAIN1980
      GO TO 8                                                           MAIN1990
  509 FORMAT(1H010X, 49HORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXEMAIN2000
     1S18X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VECMAIN2010
     2TOR8X,8HZ VECTOR)                                                 MAIN2020
  519 FORMAT(1H 10X,3E16.7,8X,3E16.7)                                   MAIN2030
  529 FORMAT(1H010X,51HORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXMAIN2040
     1ES16X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VEMAIN2050
     2CTOR8X,8HZ VECTOR)                                                MAIN2060
  539 WRITE (NOUT,509)                                                  MAIN2070
      WRITE (NOUT,519)((WRKV(J,I),I=1,3),(AAWRK(J,I),I=1,3),J           MAIN2080
     1=1,3)                                                             MAIN2090
      GO TO 8                                                           MAIN2100
C     *******PLOT CENTERING FUNCTIONS*******                            MAIN2110
  600 CALL F600                                                         MAIN2120
  601 WRITE (NOUT,609)XO(1),XO(2),SCAL1,SCAL2                           MAIN2130
  609 FORMAT(1H010X,31HORIGIN POINT IN PLOTTER COORD.(F6.2,2H ,F6.2,8H ) MAIN2140
     1 IN.  / 11X,15HOVERALL SCALE =F6.3,32H INCH/ANGSTROM ELLIPSOID SCAMAIN2150
     2LE =F6.3)                                                         MAIN2160
      GO TO 391                                                         MAIN2170
C     *******ELLIPSOID AND SYMBOL PLOT FUNCTIONS*******                 MAIN2180
C     ********FILL OUT DETAILS FOR SPECIAL MODELS********               MAIN2190
  700 GO TO (701,702,704,705,709,94),NJ3                                MAIN2200
  701 AIN(3)=8.                                                         MAIN2210
      GO TO 703                                                         MAIN2220
  702 AIN(3)=0.                                                         MAIN2230
  703 AIN(1)=4.                                                         MAIN2240
      AIN(2)=0.                                                         MAIN2250
      AIN(4)=0.                                                         MAIN2260
      GO TO 709                                                         MAIN2270
  704 AIN(1)=3.                                                         MAIN2280
      AIN(2)=-5.                                                        MAIN2290
      GO TO 706                                                         MAIN2300
  705 AIN(1)=1.                                                         MAIN2310
      AIN(2)=0.                                                         MAIN2320
  706 AIN(3)=1.                                                         MAIN2330
      AIN(4)=5.                                                         MAIN2340
  709 CALL F700                                                         MAIN2350
      GO TO 8                                                           MAIN2360
C     *******BOND FUNCTIONS*******                                      MAIN2370
  800 CALL F800                                                         MAIN2380
      GO TO 8                                                           MAIN2390
C     *******TITLE FUNCTIONS*******                                     MAIN2400
  900 CALL F900                                                         MAIN2410
      GO TO 8                                                           MAIN2420
C     *******CELL OUTLINE FUNCTIONS*******                              MAIN2430
 1000 CALL F1000                                                        MAIN2440
      GO TO 8                                                           MAIN2450
C     *******SAVE SEQUENCE FUNCTIONS*******                             MAIN2460
 1100 IF(NJ2-2)1101,1102,1103                                           MAIN2470
 1101 ISAVE=1                                                           MAIN2480
      GO TO 1104                                                        MAIN2490
 1102 ISAVE=0                                                           MAIN2500
      J=-1                                                              MAIN2510
      END FILE NSR                                                      MAIN2520
      GO TO 1104                                                        MAIN2530
 1103 ISAVE=-1                                                          MAIN2540
 1104 REWIND NSR                                                        MAIN2550
      GO TO 8                                                           MAIN2560
C     ***** TERMINATE PLOTTER TAPE IF NECESSARY *****                  MAIN2570
 3000 IF(LTNO)3005,3010,3005                                            MAIN2580
 3005 AIN(1)=-.000001                                                   MAIN2590
      AIN(2)= 0.0                                                       MAIN2600
      NJ2=2                                                             MAIN2610
      CALL F200                                                         MAIN2620
 3010 CALL EXIT                                                         MAIN2630
      STOP                                                              MAIN2640
      END                                                               MAIN2650


      FUNCTION ARCCOS(X)
C     ARCCOS(X) IN DEGREES                                              ARCC  10
      IF(1.0-ABS(X))1,2,2                                               ARCC  20
    1 X=SIGN(1.0,X)                                                     ARCC  30
    2 IF(X)3,4,5                                                        ARCC  40
    3 ARCCOS=180.0+ATAN(SQRT(1.0-X*X)/X)*57.29577951                    ARCC  50
      GO TO 6                                                           ARCC  60
    4 ARCCOS=90.0                                                       ARCC  70
      GO TO 6                                                           ARCC  80
    5 ARCCOS=ATAN (SQRT(1.0-X*X)/X)*57.29577951                         ARCC  90
    6 RETURN                                                            ARCC 100
      END                                                               ARCC 110
                                                                        ARCC 120


      SUBROUTINE ATOM(QA,Z)
C     ATOM COORDINATE SUBROUTINE                                        ATOM  10
      DIMENSION X(3),Z(3)                                               ATOM  20
      REAL*8 CHEM                                                       ATOM  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ATOM  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) ATOM  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) ATOM  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ATOM  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   ATOM  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ATOM  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     ATOM 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ATOM 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ATOM 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1ATOM 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ATOM 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ATOM 150
      K=QA/100000.0                                                     ATOM 160
      IF(K)109,109,117                                                  ATOM 170
  109 X(1)=0.0                                                          ATOM 180
      X(2)=0.0                                                          ATOM 190
      X(3)=0.0                                                          ATOM 200
      GO TO 125                                                         ATOM 210
  117 IF(K-NATOM)119,119,503                                            ATOM 220
  503 NG=5                                                              ATOM 230
      GO TO 325                                                         ATOM 240
  119 DO 123 J=1,3                                                      ATOM 250
  123 X(J)=P(J,K)                                                       ATOM 260
  125 TA=ABS(QA)                                                        ATOM 270
      KSYM=AMOD(TA,100000.0)                                            ATOM 280
      KT=KSYM/100                                                       ATOM 290
      KS=KSYM-100*KT                                                    ATOM 300
      IF(KS-NSYM)203,203,403                                            ATOM 310
  403 NG=4                                                              ATOM 320
      GO TO 325                                                         ATOM 330
  203 IF(KS)403,205,213                                                 ATOM 340
  205 Z(1)=X(1)                                                         ATOM 350
      Z(2)=X(2)                                                         ATOM 360
      Z(3)=X(3)                                                         ATOM 370
      GO TO 311                                                         ATOM 380
  213 DO 223 K=1,3                                                      ATOM 390
      Z(K)=TS(K,KS)                                                     ATOM 400
      DO 223 J=1,3                                                      ATOM 410
  223 Z(K)=Z(K)+FS(J,K,KS)*X(J)                                         ATOM 420
  311 IF(KT)403,325,313                                                 ATOM 430
  313 IF(KT-555)317,315,317                                             ATOM 440
  315 KSYM=KS                                                           ATOM 450
      GO TO 325                                                         ATOM 460
  317 K1=KT/100                                                         ATOM 470
                                                                        ATOM 480
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      K=KT-100*K1                                                       ATOM 490
      K2=K/10                                                           ATOM 500
      K3=K-10*K2                                                        ATOM 510
      Z(1)=Z(1)+FLOAT(K1-5)                                             ATOM 520
      Z(2)=Z(2)+FLOAT(K2-5)                                             ATOM 530
      Z(3)=Z(3)+FLOAT(K3-5)                                             ATOM 540
  325 RETURN                                                            ATOM 550
      END                                                               ATOM 560

      SUBROUTINE AXEQB(A1,X,B1,JJJ)                                     AXEQ  10
C     ***** SOLUTION OF MATRIX EQUATION AX=B FOR X *****                AXEQ  20
C     ***** USES METHOD OF TRIANGULAR ELIMINATION *****                 AXEQ  30
C     ***** B AND X HAVE DIMENSIONS (3,JJJ),A IS ALWAYS (3,3)           AXEQ  40
C     ***** TO INVERT A MAKE B 3 BY 3 IDENITY MATRIX *****              AXEQ  50
      DIMENSION A1(3,3),A(3,3),B(3,3),B1(3,3),X(3,3)                    AXEQ  60
      NV=JJJ                                                            AXEQ  70
C     ***** TRANSFER DATA *****                                         AXEQ  80
      DO 2 I=1,3                                                        AXEQ  90
      DO 2 J=1,3                                                        AXEQ 100
      IF(NV-J) 2,1,1                                                    AXEQ 110
    1 B(I,J)=B1(I,J)                                                    AXEQ 120
    2 A(I,J)=A1(I,J)                                                    AXEQ 130
C     ***** TRIANGULARIZE MATRIX A *****                                AXEQ 140
      DO 17 I=1,2                                                       AXEQ 150
      S=0.0                                                             AXEQ 160
      DO 4 J=I,3                                                        AXEQ 170
      R=ABS(A(J,I))                                                     AXEQ 180
      IF(R-S)4,3,3                                                      AXEQ 190
    3 S=R                                                               AXEQ 200
      L=J                                                               AXEQ 210
    4 CONTINUE                                                          AXEQ 220
      IF(L-I)5,10,5                                                     AXEQ 230
    5 DO 6 J=I,3                                                        AXEQ 240
      S=A(I,J)                                                          AXEQ 250
      A(I,J)=A(L,J)                                                     AXEQ 260
    6 A(L,J)=S                                                          AXEQ 270
      DO 8 J=1,NV                                                       AXEQ 280
      S=B(I,J)                                                          AXEQ 290
      B(I,J)=B(L,J)                                                     AXEQ 300
    8 B(L,J)=S                                                          AXEQ 310
   10 TEM=A(I,I)                                                        AXEQ 320
      IF(TEM)11,17,11                                                   AXEQ 330
   11 IPO=I+1                                                           AXEQ 340
      DO 16 J=IPO,3                                                     AXEQ 350
      IF(A(J,I))12,16,12                                                AXEQ 360
   12 S=A(J,I)/TEM                                                      AXEQ 370
      A(J,I)=0.0                                                        AXEQ 380
      DO 13 K=IPO,3                                                     AXEQ 390
   13 A(J,K)=A(J,K)-A(I,K)*S                                            AXEQ 400
      DO 15 K=1,NV                                                      AXEQ 410
   15 B(J,K)=B(J,K)-B(I,K)*S                                            AXEQ 420
   16 CONTINUE                                                          AXEQ 430
   17 CONTINUE                                                          AXEQ 440
C     ***** MODIFY SINGULAR MATRIX *****                                AXEQ 450
      DO 20 I=1,3                                                       AXEQ 460
      IF(A(I,I))20,19,20                                                AXEQ 470
   19 A(I,I)=AMAX1(1.E-25,AMAX1(A(1,1),A(2,2),A(3,3))*1.E-15)           AXEQ 480
   20 CONTINUE                                                          AXEQ 490
      DO 24 K=1,NV                                                      AXEQ 500
      DO 24 I=1,3                                                       AXEQ 510
      N=4-I                                                             AXEQ 520
      M=N+1                                                             AXEQ 530
      TEM=B(N,K)                                                        AXEQ 540
      IF(3-M)23,21,21                                                   AXEQ 550
   21 DO 22 J=M,3                                                       AXEQ 560
   22 TEM=TEM-A(N,J)*B(J,K)                                             AXEQ 570
   23 B(N,K)=TEM/A(N,N)                                                 AXEQ 580
   24 X(N,K)=B(N,K)                                                     AXEQ 590
      RETURN                                                            AXEQ 600
      END                                                               AXEQ 610

      SUBROUTINE AXES(U,V,X,ITYPE)                                      AXES  10
C     ***** STORE THREE ORTHOGONAL VECTORS EACH 1 ANGSTROM LONG *****   AXES  20
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         AXES  30
C     *****IABS(ITYPE)=1 W(1)=U,W(2)=(UXV),W(3)=UX(UXV) *****           AXES  40
C     *****IABS(ITYPE)=2 W(1)=U,W(2)=(UXV) XU,W(3)=(UXV) *****          AXES  50
C     ***** ITYPE=0 W(1)=A,W(2)=(AXB) XA,W(3)=(AXB), ABC=CELL VECTORS ***AXES  60
      DIMENSION U(3),V(3),W(3,3),X(3,3)                                 AXES  70
      IT=ITYPE                                                          AXES  80
      IF(IT)115,105,115                                                 AXES  90
  105 U(1)=1.                                                           AXES 100
      U(2)=0.                                                           AXES 110
      U(3)=0.                                                           AXES 120
      V(1)=0.                                                           AXES 130
      V(2)=1.                                                           AXES 140
      V(3)=0.                                                           AXES 150
  115 DO 125 J=1,3                                                      AXES 160
  125 W(J,1)=U(J)                                                       AXES 170
      IF(IABS(IT)-1)145,135,145                                         AXES 180
  135 CALL NORM(U,V,W(1,2),IT)                                          AXES 190
      CALL NORM(U,W(1,2),W(1,3),IT)                                     AXES 200
      GO TO 155                                                         AXES 210
  145 CALL NORM(U,V,W(1,3),IT)                                          AXES 220
      CALL NORM(W(1,3),U,W(1,2),IT)                                     AXES 230
  155 DO 195 I=1,3                                                      AXES 240
      IF(IT)165,165,175                                                 AXES 250
  165 IC=-1                                                             AXES 260
      GO TO 195                                                         AXES 270
  175 IC=1                                                              AXES 280
  195 CALL UNIT(W(1,I),X(1,I),IC)                                       AXES 290
      RETURN                                                            AXES 300
      END                                                               AXES 310

      SUBROUTINE BOND(Z1,Z2,NB,NA1,NA2)                                 BOND  10
      DIMENSION B(3,3),E(3,3),S(3,3),U(3,3),VUE(3)                      BOND  20
      DIMENSION V7(3),W(13,2),X(3),Z(3)                                 BOND  30
      REAL*8 CHEM                                                       BOND  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    BOND  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) BOND  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) BOND  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) BOND  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   BOND  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   BOND 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     BOND 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   BOND 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD BOND 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1BOND 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   BOND 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                BOND 160
C     ***** OBTAIN POSITIONAL PARAMETERS *****                          BOND 170
      NG1=0                                                             BOND 180
      DO 105 J=1,26                                                     BOND 190
  105 W(J,1)=0.                                                         BOND 200
      W(1,1)=Z1                                                         BOND 210
      W(1,2)=Z2                                                         BOND 220
      DO 135 I=1,2                                                      BOND 230
      CALL XYZ(W(1,I),W(4,I),2)                                         BOND 240
      IF(NG)125,110,125                                                 BOND 250
  110 DO 115 J=1,3                                                      BOND 260
  115 W(J+6,I)=XT(J)                                                    BOND 270
      K=W(1,I)/100000.                                                  BOND 280
      L=W(1,I)-FLOAT(K)*100000.                                         BOND 290
      CALL PLTXY(W(4,I),W(2,I))                                         BOND 300
      IF(EDGE-BRDR*.25)120,128,128                                      BOND 310
  120 NG=10                                                             BOND 320
  125 NG1=1                                                             BOND 330
      WRITE (NOUT,136)CHEM(K),K,L,(W(J,I),J=2,9)                        BOND 340
      CALL ERPNT(W(1,I),800)                                            BOND 350
      GO TO 135                                                         BOND 360
  128 IF(NJ2-10)130,135,135                                             BOND 370
  130 WRITE (NOUT,136)CHEM(K),K,L,(W(J,I),J=2,9)                        BOND 380
  135 CONTINUE                                                          BOND 390
  136 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)   2F8.2,5X,3F8.3,13X,3F8.4)    BOND 400
      IF(NG1)999,140,999                                                BOND 410
  140 CALL DIFV(W(7,1),W(7,2),V7)                                       BOND 420
      DIST=SQRT(VMV(V7,AA,V7))                                          BOND 430
      IF(MOD(NJ2,10)-3)143,142,142                                      BOND 440
  142 HGT=SCL*.12                                                       BOND 450
      CALL SIMBOL(W(2,1),W(3,1),HGT,MOD(IFIX(W(1,1)/100000.),10),0.,-   BOND 460
     11)                                                                BOND 470
      CALL SIMBOL(W(2,2),W(3,2),HGT,MOD(IFIX(W(1,2)/100000.),10),0.,-   BOND 480
     12)                                                                BOND 490
      GO TO 570                                                         BOND 500
  143 KODE=KD(5,NB)                                                     BOND 510
      IF(KODE)145,144,146                                               BOND 520
  144 NBND=0                                                            BOND 530
      GO TO 148                                                         BOND 540
  145 KODE=-KODE                                                        BOND 550
  146 NBND=128/2**KODE                                                  BOND 560
C     ***** FIND UPPERMOST ATOM PUT IN POSITION ONE *****               BOND 570
  148 IF(VIEW)152,150,152                                               BOND 580
  150 W(12,1)=1.                                                        BOND 590
      W(12,2)=1.                                                        BOND 600
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      IF(W(6,1)-W(6,2)) 165,175,175
C     *****VECTOR FROM ATOM TO VIEWPOINT *****
  152 DO 160 I=1,2
      DO 155 J=10,12
  155 W(J,I)=-W(J-6,I)
      W(12,I)=W(12,I)+VIEW
C     ***** DISTANCE SQUARED TO VIEWPOINT *****
  160 W(13,I)=VV(W(10,I),W(10,I))
      IF(W(13,2)-W(13,1)) 165,175,175
C     ***** SWITCH ATOMS *****
  165 DO 170 J=1,13
      T1=W(J,1)
      W(J,1)=W(J,2)
  170 W(J,2)=T1
C     ***** FORM IDEMFACTOR MATRIX *****
  175 DO 180 J=1,3
      E(J,J)=1.
      E(J+1,1)=0.
  180 E(J+5,1)=0.
C     ***** FORM VECTOR SET RADIAL TO BOND *****
      CALL DIPV(W(4,2),W(4,1),DA(1,3))
      CALL UNIT(DA(1,3),V3,1)
C     ***** UNIT VECTOR FROM BOND MIDPOINT TO REFERENCE VIEWPOINT *****
      DO 183 I=1,3
      V2(I)=0.0
      DO 181 J=1,3
  181 V2(I)=V2(I)+AABEV(J,3)*WRKV(J,I)
      IF(VIEW) 183,183,182
  182 V2(I)=V2(I)*VIEW-0.5*(W(I+3,1)+W(I+3,2))
  183 CONTINUE
      CALL UNIT(V2,V2,1)
      T6=ABS(VV(V3,V2))
      IF(.9994-T6) 185,185,187
C     ***** ALTERNATE CALC IF BOND IS ALONG REFERENCE VIEW DIRECTION ***
  185 DO 186 J=1,3
  186 V2(J)=W(J+9,1)+W(J+9,2)
      CALL UNIT(V2,V2,1)
      T6=ABS(VV(V3,V2))
      IF(.9994-T6) 390,390,187
  187 CALL AXES(V3,V2,B,1)
  188 T1=CD(3,NB)/SCAL2
      DO 190 J=1,3
      DA(J,1)=-B(J,2)*T1
  190 DA(J,2)=-B(J,3)*T1
      IF(NBND) 500,500,195
  195 CALL RADIAL(3)
C     ***** DERIVE QUADRICS FOR EACH ATOM *****
      DO 380 II=1,2
      CALL PAXES(W(1,II),2)
      IF(NG) 205,210,205
  205 CALL ERPNT(W(1,II),800)
      GO TO 999
C     ***** DOES BOND GO TO ELLIPSOID OR TO ENVELOPE *****
  210 T1=3-II*2
      DO 212 J=1,3
      V3(J)=V3(J)*T1
  212 VUE(J)=0.
      IF(KD(5,NB)) 260,260,215
  215 IF(VMV(V3,Q,W(10,II))) 220,260,260
  220 IBND=0
      IF(VIEW) 240,240,225
C     ***** DERIVE TANGENT CONE DIRECTLY WITHOUT ROTATING COORDINATES **
  225 T2=-(SCAL2*RMS(1)*RMS(2)*RMS(3))**2
      DO 230 J=1,3
      V1(J)=-W(J+9,II)/SCAL1
      VUE(J)=V1(J)/SCAL2
C     ***** INVERT ELLIPSOID MATRIX *****
      DO 230 K=J,3
      T1=0.0
      DO 228 I=1,3
  228 T1=T1+PAC(J,I)*PAC(K,I)*RMS(I)**2
      U(J,K)=T1
  230 U(K,J)=T1
C     *****  ADD POLARIZED COFACTOR MATRIX TO ELLIPSOID MATRIX *****
      DO 235 J=1,3
      J1=MOD(J,3)+1
      VJ1=V1(J1)
      J2=MOD(J+1,3)+1
      VJ2=V1(J2)
      DO 235 K=J,3
      K1=MOD(K,3)+1
      K2=MOD(K+1,3)+1
      S(J,K)=T2*Q(J,K)+(VJ2*(U(J1,K1)*V1(K2)-U(J1,K2)*V1(K1))
     1                 + VJ1*(U(J2,K2)*V1(K1)-U(J2,K1)*V1(K2)))
  235 S(K,J)=S(J,K)
      T5=0.0
      GO TO 300
C     ***** DERIVE TANGENT CYLINDER WITH AXIS ALONG Z *****
  240 T1=-1.0/Q(3,3)
      DO 250 J=1,2
      DO 245 K=1,2
  245 S(K,J)=Q(K,J)+Q(K,3)*Q(J,3)*T1
      S(3,J)=0.0
  250 S(J,3)=0.0
      S(3,3)=0.0
      GO TO 270
C     ***** TRANSFER ELLIPSOID *****
  260 DO 265 J=1,9
  265 S(J,1)=Q(J,1)
      IBND=II
  270 T5=1.
C     ***** CHECK FOR BOND TAPER *****
  300 IF(II-2) 305,310,310
  305 RADIUS=1.+T6*TAPER
      GO TO 320
  310 RADIUS=1.-T6*TAPER
  320 CALL MV(S,V3,V4)
      T2=VV(V3,V4)
C     ***** COMPUTE BOND INTERSECTION *****
      KL=5-II-II
      KSTP=4
      IF(NJ2-21) 324,322,322
  322 KSTP=32
  324 DO 335 K=1,65,KSTP
      DO 325 J=1,3
      V6(J)=D(J,K)*RADIUS
  325 V5(J)=V6(J)+VUE(J)
      T3=VV(V5,V4)
      T4=T3*T3-T2*(VMV(V5,S,V5)-T5)
      IF(T4) 345,330,330
  330 T4=SQRT(T4)
      T1=(T4-T3)/T2
      T3=(-T4-T3)/T2
      L=K+KL-1
      DO 335 J=1,3
      D(J,L)=(V6(J)+T1*V3(J))*SCL
  335 D(J,L+1)=(-V6(J)-T3*V3(J))*SCL
      IF(IBND+21-NJ2) 360,338,360
  338 IF(KD(5,NB)) 360,360,340
C     ***** FOR OVERLAP, MAKE BOND QUADRANGLE TANGENT TO ENVELOPING CONE
  340 T3=VV(VUE,V4)
      T4=T3**2-T2*(VMV(VUE,S,VUE)-T5)
      IF(T4) 345,350,350
  345 NG=13
      CALL ERPNT(W(1,II),800)
      GO TO 999
  350 T1=(SQRT(T4)-T3)/T2
      DO 355 J=1,3
      T4=(T1*V3(J)*SCL-0.5*(D(J,KL)+D(J,KL+64)))*1.001
      D(J,KL)=D(J,KL)+T4
  355 D(J,KL+64)=D(J,KL+64)+T4
  360 CALL PROJ(D(1,KL),DP(1,II),W(4,II),XO,VIEW,1,65,KSTP)
      IF(IBND-1) 370,365,370
  365 CALL PROJ(D(1,KL+5),DP(1,II+68),W(4,II),XO,VIEW,1,61,KSTP)
      GO TO 380
C     ***** RETRACE TOP HALF *****
  370 DO 375 K=4,64,4
      L=K+II
      M=L+64
      N=66-L
      DP(1,M)=DP(1,N)
  375 DP(2,M)=DP(2,N)
  380 CONTINUE
C     ***** CHECK FOR OVERLAP OR HIDDEN BOND *****
      DO 395 K=1,65,32
      T1=0.
      T2=0.
      DO 385 J=1,2
      T1=T1+(DP(J,K)-W(J+1,1))**2
  385 T2=T2+(DP(J,K+1)-W(J+1,1))**2
      IF(T2-T1) 390,390,395
  390 NG=14
      CALL ERPNT(W(1,2),800)
      GO TO 999
  395 CONTINUE
C     ***** CALL OVERLAP ROUTINE *****
      ICQ=0
      CALL LAP800(NA1,NA2,ICQ)
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      IF (NJ2-21) 400,999,999                                           BOND2290
  400 IF (ICQ) 390,405,405                                              BOND2300
C     ***** DRAW BOND OUTLINE *****                                     BOND2310
  405 CALL DRAW(DP(1,1),0.,0.,3)                                        BOND2320
      DO 415 K=5,129,4                                                  BOND2330
  415 CALL DRAW(DP(1,K),0.,0.,2)                                        BOND2340
      DO 420 K=2,66,4                                                   BOND2350
  420 CALL DRAW(DP(1,K),0.,0.,2)                                        BOND2360
      CALL DRAW(DP(1,65),0.,0.,2)                                       BOND2370
C     ***** DRAW BOND DETAIL *****                                      BOND2380
  425 K=65                                                              BOND2390
  430 K=K-NBND                                                          BOND2400
      IF (K-1) 500,500,435                                              BOND2410
  435 CALL DRAW(DP(1,K),0.,0.,3)                                        BOND2420
      CALL DRAW(DP(1,K+1),0.,0.,2)                                      BOND2430
      K=K-NBND                                                          BOND2440
      IF (K-1) 500,500,440                                              BOND2450
  440 CALL DRAW(DP(1,K+1),0.,0.,3)                                      BOND2460
      CALL DRAW(DP(1,K),0.,0.,2)                                        BOND2470
      GO TO 430                                                         BOND2480
  500 HGT=CD(4,NB)                                                      BOND2490
      OFF=CD(5,NB)                                                      BOND2500
      IF (HGT) 570,570,510                                              BOND2510
C     ***** PERSPECTIVE BOND LABEL ROUTINE *****                        BOND2520
C     ***** BASE DECISIONS ON REFERENCE SYSTEM *****                    BOND2530
  510 K=0                                                               BOND2540
      CALL DIFV(W(7,2),W(7,1),V7)                                       BOND2550
      CALL VM(V7,AAREV,V1)                                              BOND2560
      CALL AXES(V1,E(1,3),U,1)                                          BOND2570
      DO 535 I=1,3                                                      BOND2580
      T1=1.                                                             BOND2590
      IF (I-2) 515,515,520                                              BOND2600
  515 IF (VV(U(1,I),SYMB(1,I))) 525,530,530                             BOND2610
  520 IF (MOD(K,2)) 530,525,530                                         BOND2620
  525 T1=-1.                                                            BOND2630
      K=K+1                                                             BOND2640
  530 DO 535 J=1,3                                                      BOND2650
      U(J,I)=U(J,I)*T1                                                  BOND2660
  535 VT(J,I)=B(J,I)*T1                                                 BOND2670
      DO 540 J=1,3                                                      BOND2680
  540 VT(J,4)=.5*(W(J+3,1)+W(J+3,2))                                    BOND2690
C     ***** CHECK FOR EXCESS FORESHORTENING *****                       BOND2700
      IF (FORE-ABS(U(3,1))) 545,550,550                                 BOND2710
  545 CALL NORM(U(1,2),SYMB(1,3),VT(1,1),1)                             BOND2720
      VT(1,3)=SYMB(1,3)                                                 BOND2730
      VT(2,3)=SYMB(2,3)                                                 BOND2740
      VT(3,3)=SYMB(3,3)                                                 BOND2750
      HGT=CD(6,NB)                                                      BOND2760
      OFF=CD(7,NB)                                                      BOND2770
      IF (HGT) 550,999,550                                              BOND2780
  550 T1=CD(8,NB)                                                       BOND2790
      Z(1)=VT(1,4)-HGT*(11.+3.*T1)/7.                                   BOND2800
      Z(2)=VT(2,4)+OFF-HGT*.5                                           BOND2810
      Z(3)=VT(3,4)                                                      BOND2820
      XO(3)=Z(3)                                                        BOND2830
      ITILT=1                                                           BOND2840
      I9=T1+2.                                                          BOND2850
      T9=10.**I9                                                        BOND2860
      DISTR=AINT((DIST*T9)+0.5)/T9 +.0001                               BOND2870
      CALL NUMBUR(Z(1),Z(2),HGT,DISTR,0.,I9)                            BOND2880
  570 ITILT=0                                                           BOND2890
      IF (NJ2-10) 580,999,999                                           BOND2900
  580 WRITE (NOUT,571) DIST                                             BOND2910
  571 FORMAT(1H 59X,10HDISTANCE =F8.3/1H )                              BOND2920
  999 RETURN                                                            BOND2930
      END                                                               BOND2940


      SUBROUTINE DIFV(X,Y,Z)                                            DIFV  10
C     VECTOR - VECTOR                                                   DIFV  20
C     Z(3)=X(3)-Y(3)                                                    DIFV  30
      DIMENSIONX(3),Y(3),Z(3)                                           DIFV  40
      DO 111 I=1,3                                                      DIFV  50
  111 Z(I)=X(I)-Y(I)                                                    DIFV  60
      RETURN                                                            DIFV  70
      END                                                               DIFV  80


      SUBROUTINE DRAW(W,DX,DY,NPEN)                                     DRAW  10
      DIMENSION W(3),X(3),Y(3),Z(3)                                     DRAW  20
      REAL*8 CHEM                                                       DRAW  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    DRAW  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) DRAW  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) DRAW  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REPV(3,3) DRAW  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   DRAW  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   DRAW  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     DRAW 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   DRAW 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD DRAW 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REPV,RES,RMS,SCAL1DRAW 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   DRAW 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                DRAW 150
      Y(1)=W(1)+DX                                                      DRAW 160
      Y(2)=W(2)+DY                                                      DRAW 170
      IF (ITILT) 115,140,115                                            DRAW 180
C     ***** ROTATE FOR PERSPECTIVE TITLE *****                          DRAW 190
  115 Y(3)=XO(3)                                                        DRAW 200
      DO 120 I=1,3                                                      DRAW 210
  120 Z(I)=Y(I)-VT(I,4)                                                 DRAW 220
      DO 130 I=1,3                                                      DRAW 230
  130 X(I)=VT(I,1)*Z(1)+VT(I,2)*Z(2)+VT(I,3)*Z(3)+VT(I,4)               DRAW 240
      CALL PLTXY(X,Y)                                                   DRAW 250
C     ***** CHECK BOUNDRY *****                                         DRAW 260
  140 DO 160 J=1,2                                                      DRAW 270
      IF (Y(J)-XLNG(J)+.1) 150,150,145                                  DRAW 280
  145 Y(J)=XLNG(J)-.1                                                   DRAW 290
  150 IF (Y(J)-.1) 155,160,160                                          DRAW 300
  155 Y(J)=.1                                                           DRAW 310
  160 CONTINUE                                                          DRAW 320
C     ***** CHECK FOR OVERLAP *****                                     DRAW 330
      NCQ=0                                                             DRAW 340
      CALL LAPDRW(Y,NPEN,NCQ)                                           DRAW 350
      IF (NCQ) 165,165,170                                              DRAW 360
C     ***** CALL PLOTTING ROUTINE IF NO OVERLAPPING ELEMENTS ARE STORED DRAW 370
  165 CALL SCRIBE(Y,NPEN,LTNO)                                          DRAW 380
  170 RETURN                                                            DRAW 390
      END                                                               DRAW 400


      SUBROUTINE EIGEN (W,VALU,VECT)                                    EIGE  10
C     ***** EIGENVALUES AND EIGENVECTORS OF 3X3 MATRIX *****            EIGE  20
      DIMENSION W(3,3),VALU(3),VECT(3,3),A(3,3),B(3,3),V(3),U(3)        EIGE  30
      COMMON NG                                                         EIGE  40
C     ***** STATEMENT FUNCTION *****                                    EIGE  50
      PHIF(Z)=((B2-Z)*Z+B1)*Z+B0                                        EIGE  60
C     ***** START OF PROGRAM *****                                      EIGE  70
      ERRND=5.E-7                                                       EIGE  80
      SIGMA=0.                                                          EIGE  90
      DO 115 J=1,3                                                      EIGE 100
      DO 115 I=1,3                                                      EIGE 110
      TEM=W(I,J)                                                        EIGE 120
      A(I,J)=TEM                                                        EIGE 130
  115 SIGMA=SIGMA+TEM*TEM                                               EIGE 140
C     ***** CHECK FOR NULL MATRIX *****                                 EIGE 150
      IF (SIGMA) 230,230,120                                            EIGE 160
  120 SIGMA=SQRT(SIGMA)                                                 EIGE 170
C     ***** FORM CHARACTERISTIC EQUATION *****                          EIGE 180
      B2=A(1,1)+A(2,2)+A(3,3)                                           EIGE 190
      B1=-A(1,1)*A(2,2)-A(1,1)*A(3,3)-A(2,2)*A(3,3)+A(1,3)*A(3,1)       EIGE 200
     1+A(2,3)*A(3,2)+A(1,2)*A(2,1)                                      EIGE 210
      B0=A(1,1)*A(2,2)*A(3,3)+A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(3,2)*A(2,1)-EIGE 220
     1A(1,3)*A(3,1)*A(2,2)-A(1,1)*A(2,3)*A(3,2)-A(1,2)*A(2,1)*A(3,3)    EIGE 230
C     ***** FIRST ROOT BY BISECTION *****                               EIGE 240
      X=0.                                                              EIGE 250
      Y=SIGMA                                                           EIGE 260
      TEM=PHIF(SIGMA)                                                   EIGE 270
      VNEW=0.0                                                          EIGE 280
      IF (B0) 135,250,145                                               EIGE 290
  135 IF (TEM) 140,140,165                                              EIGE 300
  140 Y=-Y                                                              EIGE 310
      GO TO 165                                                         EIGE 320
  145 Y=0.                                                              EIGE 330
      X=SIGMA                                                           EIGE 340
      IF (TEM) 165,165,150                                              EIGE 350
  150 X=-X                                                              EIGE 360
C     ***** NOW PHIF(X).LT.0.AND.PHIF(Y).GT.0. *****                    EIGE 370
  165 VNEW=(X+Y)*.5                                                     EIGE 380
      DO 225 I=1,40                                                     EIGE 390
  175 IF (PHIF(VNEW)) 180,250,185                                       EIGE 400
  180 X=VNEW                                                            EIGE 410
      GO TO 200                                                         EIGE 420
  185 Y=VNEW                                                            EIGE 430
  200 VOLD=VNEW                                                         EIGE 440
      VNEW=(X+Y)*.5                                                     EIGE 450
      TEM=ABS(VOLD-VNEW)                                                EIGE 460
      IF (TEM-ERRND) 250,250,205                                        EIGE 470
  205 IF (VOLD) 210,225,210                                             EIGE 480
```

```
  210 IF (ABS(TEM/VOLD)-ERRND) 250,250,225
  225 CONTINUE
C     ***** DID NOT CONVERGE, SET ERROR INDICATOR *****
  230 NG=6
      GO TO 400
C     ***** STORE FIRST ROOT *****
  250 U(3)=VNEW
C     ***** DEFLATE *****
      C1=B2-VNEW
      C0=B1+C1*VNEW
C     ***** SOLVE QUADRATIC *****
      TEM=C1*C1+4.*C0
      IF(TEM) 255,265,260
C     ***** IGNORE IMAGINARY COMPONENT OF COMPLEX ROOT *****
  255 TEM=0.
      GO TO 265
  260 TEM=SQRT(TEM)
  265 U(1)=.5*(C1-TEM)
      U(2)=.5*(C1+TEM)
C     ***** SORT ROOTS *****
      DO 275 J=1,2
      IF(U(J)-U(3)) 275,275,270
  270 TEM=U(J)
      U(J)=U(3)
      U(3)=TEM
  275 CONTINUE
      LLL=-2
      DO 375 III=1,2
C     ***** CHECK FOR MULTIPLE ROOTS *****
      TEM=ERRND*100.
      NG=0
      L=1
      DO 305 I=1,2
      IF(U(I+1)-U(I)-TEM) 300,300,290
  290 IF(U(I)) 295,305,295
  295 IF(ABS((U(I+1)-U(I))/U(I))-TEM) 300,300,305
  300 L=L-1
      NG=NG-2*I
  305 CONTINUE
      IF(LLL-L) 308,400,400
  308 LLL=L
C     ***** EIGENVECTOR ROUTINE *****
      DO 375 II=1,3
      T1=U(II)
      IF(L) 315,310,322
C     ***** TWO VECTORS NULL FOR DOUBLE ROOT *****
  310 IF(NG+5-II) 315,322,315
C     ***** ALL VECTORS NULL FOR TRIPLE ROOT *****
  315 DO 320 J=1,3
  320 VECT(J,II)=0.0
      GO TO 375
  322 DO 325 J=1,3
  325 A(J,J)=W(J,J)-T1
      SMAX=0.0
      DO 355 I=1,3
      I1=1
      IF(I-2) 335,335,340
  335 I1=I+1
  340 B(I,1)=A(I,2)*A(I1,3)-A(I,3)*A(I1,2)
      B(I,2)=A(I,3)*A(I1,1)-A(I,1)*A(I1,3)
      B(I,3)=A(I,1)*A(I1,2)-A(I,2)*A(I1,1)
      TEM=B(I,1)**2+B(I,2)**2+B(I,3)**2
      IF(TEM-SMAX) 355,355,350
  350 SMAX=TEM
      IMAX=I
  355 CONTINUE
      IF(SMAX) 353,353,360
  353 NG=7
      GO TO 375
  360 SMAX=SQRT(SMAX)
      DO 365 J=1,3
  365 V(J)=B(IMAX,J)/SMAX
C     ***** REFINE EIGENVECTOR *****
      CALL AXEQB(A,V,V,1)
      TEM=AMAX1(ABS(V(1)),ABS(V(2)),ABS(V(3)))
      DO 370 J=1,3
  370 V(J)=V(J)/TEM
      CALL UNIT(V,VECT(1,II),1)
C     ***** REFINE EIGENVALUE *****
      T1=VMV(VECT(1,II),W,VECT(1,II))
      U(II)=T1
  375 VALU(II)=T1
  400 RETURN
      END
```

```
EIGE 490
EIGE 500
EIGE 510
EIGE 520
EIGE 530
EIGE 540
EIGE 550
EIGE 560
EIGE 570
EIGE 580
EIGE 590
EIGE 600
EIGE 610
EIGE 620
EIGE 630
EIGE 640
EIGE 650
EIGE 660
EIGE 670
EIGE 680
EIGE 690
EIGE 700
EIGE 710
EIGE 720
EIGE 730
EIGE 740
EIGE 750
EIGE 760
EIGE 770
EIGE 780
EIGE 790
EIGE 800
EIGE 810
EIGE 820
EIGE 830
EIGE 840
EIGE 850
EIGE 860
EIGE 870
EIGE 880
EIGE 890
EIGE 900
EIGE 910
EIGE 920
EIGE 930
EIGE 940
EIGE 950
EIGE 960
EIGE 970
EIGE 980
EIGE 990
EIGE1000
EIGE1010
EIGE1020
EIGE1030
EIGE1040
EIGE1050
EIGE1060
EIGE1070
EIGE1080
EIGE1090
EIGE1100
EIGE1110
EIGE1120
EIGE1130
EIGE1140
EIGE1150
EIGE1160
EIGE1170
EIGE1180
EIGE1190
EIGE1200
EIGE1210
EIGE1220
EIGE1230
EIGE1240
EIGE1250
EIGE1260
EIGE1270
EIGE1280
EIGE1290
EIGE1300
EIGE1310
EIGE1320
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      SUBROUTINE ERPNT(T1,N)                                            ERPN  10
      REAL*8 CHEM                                                       ERPN  20
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ERPN  30
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) ERPN  40
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) ERPN  50
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ERPN  60
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   ERPN  70
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ERPN  80
      DIMENSION XLNG(3),XO(3),XT(3)                                     ERPN  90
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ERPN 100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ERPN 110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1ERPN 120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ERPN 130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ERPN 140
      WRITE (NOUT,115)NG,T1,N                                           ERPN 150
  115 FORMAT(1H 10X,10HFAULT NG =I3,F10.0,I6/1H )                       ERPN 160
      NG=0                                                              ERPN 170
      RETURN                                                            ERPN 180
      END                                                               ERPN 190


      SUBROUTINE F200                                                   F200  10
      DIMENSION HEADER(4),PLA(3000)                                     F200  20
      DATA HEADER/3*4H    ,4H$   /,ZERO/0.0/                             F200  30
      REAL*8 CHEM                                                       F200  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F200  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F200  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F200  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F200  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F200  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F200 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F200 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F200 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F200 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F200 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F200 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F200 160
C     ***** CALCOMP CONTROL *****                                       F200 170
      NJQ = NJ2+1                                                       F200 180
      GO TO(260,200,225,205,210,260),NJQ                                F200 190
C     ***** INITIATE MECHANICAL CALCOMP PLOTTER (201 INSTRUCTION) ***** F200 200
  200 LTNO = 15                                                         F200 210
      CALL PLOTS(PLA,3000,LTNO)                                         F200 220
      GO TO 260                                                         F200 230
C     ***** INITIATE C.R.T. CALCOMP PLOTTER (203 INSTRUCTION) *****     F200 240
  205 LTNO = -99                                                        F200 250
      CALL JOBNUM(HEADER(1))                                            F200 260
      CALL IDAY(HEADER(2))                                              F200 270
      CALL CRT(PLA,3000,HEADER,0)                                       F200 280
C     ***** SET C.R.T. X,Y ORIGIN AND BEAM INTENSITY BASELINE *****     F200 290
      IZ = AIN(3)                                                       F200 300
      CALL CRT(AIN(1),AIN(2),IZ,3)                                      F200 310
      GO TO 215                                                         F200 320
C     ***** RESET BEAM INTENSITY (204 INSTRUCTION) *****                F200 330
  210 IZ = AIN(1)                                                       F200 340
      IF(IZ) 215,215,220                                                F200 350
  215 IZ = 18                                                           F200 360
  220 CALL CRT(ZERO,ZERO,IZ,7)                                          F200 370
      GO TO 260                                                         F200 380
C     ***** TERMINATE THE PLOT AND ADVANCE PLOTTER (202 INSTRUCTION) ***F200 390
  225 IF(LTNO) 235,260,230                                              F200 400
  230 CALL PLOT(AIN(1),AIN(2),-3)                                       F200 410
      GO TO 260                                                         F200 420
C     ***** THE FOLLOWING ARE FOR CRT FILM ADVANCE ETC. *****           F200 430
  235 IF(AIN(1)) 245,240,250                                            F200 440
C     ***** ADD BLOCK ADDRESS BUT DO NOT ADVANCE CRT FILM *****         F200 450
  240 IB = 1000                                                         F200 460
      GO TO 255                                                         F200 470
C     ***** ADVANCE CRT FILM AND CLOSE OUTPUT TAPE FILE ****            F200 480
  245 IB = 9000                                                         F200 490
      GO TO 255                                                         F200 500
C     ***** ADD BLOCK ADDRESS AND ADVANCE CRT FILM *****                F200 510
  250 IB = 0000                                                         F200 520
C     ***** IDENTIFICATION TITLE FRAME BETWEEN PLOTS *****              F200 530
      CALL CRT(ZERO,ZERO,IB,2)                                          F200 540
      CALL SIMBOL(0.2,0.0,0.25,TITLE(1),40.,72)                         F200 550
  255 CALL CRT(ZERO,ZERO,IB,2)                                          F200 560
  260 RETURN                                                            F200 570
      END                                                               F200 580


      SUBROUTINE F400                                                   F400  10
C     ***** ATOM LIST FUNCTIONS *****                                   F400  20
      REAL*8 CHEM                                                       F400  30
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      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      NG=0
      IF(LATM)402,402,400
  400 DO 401 I=1,LATM
  401 CALL ATOM(ATOMS(1,I),ATOMS(2,I))
  402 IF(MOD(NJ2,10)-1)499,404,403
  403 CALL SEARC
      GO TO 499
C     ***** STORES (401) OR REMOVES (411) RUNS OF ATOMS *****
C     ***** RUN HIERARCHY = ATOM NO./SYM/ A/B/C TRANS. *****
  404 II=1
C     ***** FIND RUNS IN AIN ARRAY *****
  405 T1=AIN(II)
      IF(T1)410,410,420
  410 II=II+1
      IF(140-II)499,405,405
  420 JJ=II
C     ***** SET INITIAL RUN VALUES *****
      M1=T1/100000.
      M2=AMOD(T1,100.)
      M5=AMOD(T1/100.,1000.)
      IF(M5)422,422,423
  422 M5=555
  423 M3=M5/100
      M4=MOD(M5/10,10)
      M5=MOD(M5,10)
  425 JJ=JJ+1
      IF(140-JJ)435,430,430
  430 T2=-AIN(JJ)
      IF(T2)435,425,440
  435 II=JJ-1
C     ***** SET TERMINAL VALUES FOR DEGENERATE RUN *****
      N1=M1
      N2=M2
      N3=M3
      N4=M4
      N5=M5
      GO TO 450
  440 II=JJ
C     ***** SET TERMINAL RUN VALUES *****
      N1=T2/100000.
      N2=AMOD(T2,100.)
      N5=AMOD(T2/100.,1000.)
      IF(N5)445,445,446
  445 N5=555
  446 N3=N5/100
      N4=MOD(N5/10,10)
      N5=MOD(N5,10)
C     ***** LOOP THROUGH ALL RUNS *****
  450 DO 490 L5=M5,N5
      DO 490 L4=M4,N4
      DO 490 L3=M3,N3
      DO 490 L2=M2,N2
      DO 490 L1=M1,N1
      V1(1)=FLOAT(L1)*100000.+FLOAT(L3*10000+L4*1000+L5*100+I2)
      CALL ATOM(V1(1),V1(2))
      IF(NG)455,458,455
  455 CALL ERPNT(V1(1),401)
      GO TO 490
  458 CALL STOR
  490 CONTINUE
      GO TO 410
  499 RETURN
      END


      SUBROUTINE F500
      DIMENSION RM(3,3),V(3,4)
      REAL*8 CHEM
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      NG=0
      IF(NJ2-11)500,700,710
  500 IF(NJ2-1)710,501,510
  501 T1=AIN(1)
      CALL ATOM(T1,ORGN)
      IF(NG)502,504,502
  502 CALL ERPNT(T1,501)
      CALL EXIT
  504 DO 506 K=1,4
      T1=AIN(K+1)
      CALL ATOM(T1,V(1,K))
      IF(NG)502,506,502
  506 CONTINUE
      DO 507 J=1,3
      V1(J)=V(J,2)-V(J,1)
  507 V2(J)=V(J,4)-V(J,3)
      IND=-1
      IF(AIN(7))509,509,508
  508 IND=-2
  509 CALL AXES(V1,V2,REFV,IND)
      GO TO 670
  510 IF(NJ2-4)515,511,599
C     ***** SHIFT ORIGIN FOR PROJECTION AXIS (IN INCHES) *****
  511 DO 513 J=1,3
      DO 512 K=1,3
  512 ORGN(J)=ORGN(J)+REFV(J,K)*AIN(K)/SCAL1
  513 XO(J)=XO(J)+AIN(J)
      GO TO 675
C     ***** FORM ROTATION MATRIX *****
  515 DO 552 L=1,139,2
      I=AIN(L)
      IF(I) 532,552,516
  516 X=AIN(L+1)*1.7453293E-2
      T1=COS(X)
      T2=SIN(X)
      I3=MOD(I+2,3)+1
      I1=MOD(I3,3)+1
      I2=MOD(I1,3)+1
      RM(I1,I1)=T1
      RM(I1,I2)=T2
      RM(I1,I3)=0.0
      RM(I2,I1)=-T2
      RM(I2,I2)=T1
      RM(I2,I3)=0.0
      RM(I3,I1)=0.0
      RM(I3,I2)=0.0
      RM(I3,I3)=1.0
      CALL MM(REFV,RM,V)
      IF(NJ2-3)518,525,599
  518 DO 522 J=1,3
      DO 522 I=1,3
  522 REFV(I,J)=V(I,J)
      GO TO 552
  525 DO 528 J=1,3
      DO 528 I=1,3
  528 WRKV(I,J)=V(I,J)
      GO TO 552
  532 IF(NJ2-3)535,552,599
  535 I=MOD(-I,3)
      DO 542 J=1,I
      DO 542 K=1,3
      T1=REFV(K,3)
      REFV(K,3)=REFV(K,2)
      REFV(K,2)=REFV(K,1)
  542 REFV(K,1)=T1
  552 CONTINUE
      IF(NJ2-3)670,582,599
  582 CALL MM(AA,WRKV,AAWRK)
      GO TO 699
  599 IF(NJ2-5)699,600,607
  600 IF(LATM-1)605,610,610
  605 NG=12
  606 CALL ERPNT(0.,506)
      CALL EXIT
  607 IF(NJ2-6)699,608,710
  608 IF(LATM-3)605,610,610
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  610 DO 612 J=1,3                                                      F500 920
      V2(J)=0.0                                                         F500 930
      DO 612 I=1,3                                                      F500 940
  612 RM(I,J)=0.0                                                       F500 950
      AWT=0.0                                                           F500 960
      DO 620 K=1,LATM                                                   F500 970
      CALL ATOM(ATOMS(1,K),ATOMS(2,K))                                  F500 980
      T2=1.0                                                            F500 990
      IF(NCD)618,618,613                                                F5001000
  613 I1=ATOMS(1,K)/100000.                                             F5001010
      DO 616 J=1,NCD                                                    F5001020
      T2=CD(1,J)                                                        F5001030
      IF(I1-KD(1,J))616,614,614                                         F5001040
  614 IF(KD(2,J)-I1)616,618,618                                         F5001050
  616 CONTINUE                                                          F5001060
      GO TO 620                                                         F5001070
  618 AWT=AWT+T2                                                        F5001080
      DO 619 J=1,3                                                      F5001090
  619 V2(J)=V2(J)+ATOMS(J+1,K)*T2                                       F5001100
  620 CONTINUE                                                          F5001110
      IF(AWT)605,605,621                                                F5001120
C     ***** PUT ORIGIN AT CENTER OF GRAVITY *****                       F5001130
  621 DO 622 J=1,3                                                      F5001140
  622 ORGN(J)=V2(J)/AWT                                                 F5001150
      IF(NJ2-6)699,624,710                                              F5001160
C     ***** FORM PRODUCT-MOMENT MATRIX FOR ATOMS IN ATOM LIST *****     F5001170
  624 DO 630 K=1,LATM                                                   F5001180
      T2=1.0                                                            F5001190
      IF(NCD)628,628,625                                                F5001200
  625 I1=ATOMS(1,K)/100000.                                             F5001210
      DO 627 J=1,NCD                                                    F5001220
      T2=CD(1,J)                                                        F5001230
      IF(I1-KD(1,J))627,626,626                                         F5001240
  626 IF(KD(2,J)-I1)627,628,628                                         F5001250
  627 CONTINUE                                                          F5001260
      GO TO 630                                                         F5001270
  628 DO 629 J=1,3                                                      F5001280
      T1=(ATOMS(J+1,K)-ORGN(J))*T2                                      F5001290
      DO 629 I=1,3                                                      F5001300
  629 RM(I,J)=T1*(ATOMS(I+1,K)-ORGN(I))+RM(I,J)                         F5001310
      T1=0.03/(RM(1,1)+RM(2,2)+RM(3,3))                                 F5001320
  630 CONTINUE                                                          F5001330
      DO 632 J=1,3                                                      F5001340
      DO 632 I=1,3                                                      F5001350
  632 RM(I,J)=RM(I,J)*T1                                                F5001360
C     ***** TRANSFORM TO INERTIAL AXIS SYSTEM *****                     F5001370
      CALL MM(RM,AA,DA)                                                 F5001380
      CALL EIGEN(DA,RMS,PAT)                                            F5001390
      IF(RMS(2))605,605,635                                             F5001400
  635 IF(NG)640,633,606                                                 F5001410
C     ***** MAKE SURE VECTORS ARE ORTHOGONAL --> NEW REFERENCE VECTORS *F5001420
  633 CALL AXES(PAT(1,3),PAT(1,1),REFV,-1)                              F5001430
      GO TO 665                                                         F5001440
C     ***** TWO EQUAL EIGENVECTORS SPECIAL CASE *****                   F5001450
  640 IF(NG+6)665,665,645                                               F5001460
  645 N=NG+5                                                            F5001470
      CALL UNIT(PAT(1,N),V1,-1)                                         F5001480
      DO 650 K=1,3                                                      F5001490
      IF(ABS(VMV(V1,AA,REFV(1,K)))-.58)655,650,650                      F5001500
  650 CONTINUE                                                          F5001510
  655 CALL AXES(V1,REFV(1,K),DA,-1)                                     F5001520
      DO 660 K=1,3                                                      F5001530
      L=MOD(N-K+2,3)+1                                                  F5001540
      DO 660 J=1,3                                                      F5001550
  660 REFV(J,L)=DA(J,K)                                                 F5001560
  665 NG=0                                                              F5001570
  670 CALL MM(AA,REFV,AAREV)                                            F5001580
  675 DO 680 J=1,3                                                      F5001590
      DO 680 I=1,3                                                      F5001600
      WRKV(I,J)=REFV(I,J)                                               F5001610
  680 AAWRK(I,J)=AAREV(I,J)                                             F5001620
C     ***** ELIMINATE ALL PREVIOUSLY STORED OVERLAP INFORMATION ****    F5001630
C     ***** (ALL INSTRUCTIONS FROM 501 THROUGH 510 DO THIS *****        F5001640
  699 CALL LAP500(0)                                                    F5001650
      GO TO 710                                                         F5001660
C     ***** STORE NEW OVERLAP INFORMATION (INSTRUCTION 511) *****       F5001670
  700 CALL LAP500(1)                                                    F5001680
  710 RETURN                                                            F5001690
      END                                                               F5001700
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      SUBROUTINE F600                                                   F600  10
C     ***** SCALING AND CENTERING FUNCTIONS *****                       F600  20
      DIMENSION MAX(3),SCAL(4),X(3),XMAX(3),XMIN(3),Z(2)                F600  30
      REAL*8 CHEM                                                       F600  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F600  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)F600  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F600  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F600  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F600  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F600 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F600 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F600 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD F600 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F600 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F600 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F600 160
C     ***** DEL = 1. FOR INCRUMENTING FUNCTIONS *****                   F600 170
C     ***** DEL = 0. FOR REGULAR FUNCTIONS *****                        F600 180
      DEI=FLOAT(MOD(NJ2/10,2))                                          F600 190
      NJ2=MOD(NJ2,10)                                                   F600 200
C     ***** EXPLICIT ORIGIN AND SCALE *****                             F600 210
      IF(AIN(1))602,604,602                                             F600 220
  602 XO(1)=AIN(1)+XO(1)*DEL                                            F600 230
  604 IF(AIN(2))606,608,606                                             F600 240
  606 XO(2)=AIN(2)+XO(2)*DEL                                            F600 250
  608 IF(AIN(3))612,612,609                                             F600 260
  609 IF(DEL)611,611,610                                                F600 270
  610 SCAL1=SCAL1*AIN(3)                                                F600 280
      GO TO 612                                                         F600 290
  611 SCAL1=AIN(3)                                                      F600 300
  612 IF(AIN(4))616,616,614                                             F600 310
C     ***** SET ELLIPSOID SCALE FACTOR *****                            F600 320
  614 SCAL2=AIN(4)                                                      F600 330
C     ***** AUTOMATIC ORIGIN AND/OR SCALE *****                         F600 340
  616 IF(NJ2-2)790,622,620                                              F600 350
  620 XO(1)=XLNG(1)*.5                                                  F600 360
      XO(2)=XLNG(2)*.5                                                  F600 370
  622 IF(NJ2-3)625,640,625                                              F600 380
  625 SCAL1=1.                                                          F600 390
  630 IF(LATM-1)635,635,640                                             F600 400
  635 NG=12                                                             F600 410
      CALL ERPNT(0.,602)                                                F600 420
      CALL EXIT                                                         F600 430
  640 DO 650 J=1,3                                                      F600 440
      XMAX(J)=-1.E5                                                     F600 450
  650 XMIN(J)=1.E5                                                      F600 460
C     ***** FIT BOX AROUND SET OF ATOMS *****                           F600 470
      DO 670 I=1,LATM                                                   F600 480
      CALL XYZ(ATOMS(1,I),ATOMS(2,I),3)                                 F600 490
      IF(NG)652,653,652                                                 F600 500
  652 CALL ERPNT(ATOMS(1,I),600)                                        F600 510
      GO TO 670                                                         F600 520
  653 DO 668 J=1,3                                                      F600 530
      T1=ATOMS(J+1,I)                                                   F600 540
      IF(XMAX(J)-T1)655,660,660                                         F600 550
  655 XMAX(J)=T1                                                        F600 560
      MAX(J)=I                                                          F600 570
  660 IF(T1-XMIN(J))665,668,668                                         F600 580
  665 XMIN(J)=T1                                                        F600 590
  668 CONTINUE                                                          F600 600
  670 CONTINUE                                                          F600 610
C     ***** KM=TOP ATOM *****                                           F600 620
      KM=MAX(3)                                                         F600 630
      SMULT=1.                                                          F600 640
      DO 780 M=1,5                                                      F600 650
      IF(M-2)740,675,678                                                F600 660
C     ***** CHECK VIEW DISTANCE *****                                   F600 670
  675 IF(VIEW)785,785,680                                               F600 680
  678 IF(NJ2-3)680,785,680                                              F600 690
  680 T1=ATOMS(4,KM)*SMULT                                              F600 700
      IF(VIEW*.5-T1)685,690,690                                         F600 710
C     ***** INCREASE VIEW DISTANCE *****                                F600 720
  685 VIEW=2.*T1                                                        F600 730
C     ***** FIND PERSPECTIVE PROJECTION LIMITS *****                    F600 740
  690 DO 700 J=1,2                                                      F600 750
      XMAX(J)=-1.E5                                                     F600 760
  700 XMIN(J)=1.E5                                                      F600 770
      DO 725 I=1,LATM                                                   F600 780
      DO 705 J=1,3                                                      F600 790
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  705 X(J)=ATOMS(J+1,I)*SMULT                                          F600 800
      T2=VIEW/(VIEW-X(3))                                              F600 810
      DO 725 J=1,2                                                     F600 820
      T1=X(J)*T2                                                       F600 830
      IF(XMAX(J)-T1)710,715,715                                        F600 840
  710 XMAX(J)=T1                                                       F600 850
  715 IF(T1-XMIN(J))720,725,725                                        F600 860
  720 XMIN(J)=T1                                                       F600 870
  725 CONTINUE                                                         F600 880
C     ***** REFINE PARAMETERS *****                                    F600 890
  740 IF(NJ2 -3)745,742,755                                            F600 900
  742 SMUL2=1.                                                         F600 910
      GO TO 765                                                        F600 920
C     ***** AUTOMATIC SCALE ONLY *****                                 F600 930
  745 DO 750 J=1,2                                                     F600 940
      T2=XO(J)                                                         F600 950
      SCAL(J)=(BRDR-T2)/XMIN(J)                                        F600 960
  750 SCAL(J+2)=(XLNG(J)-BRDR-T2)/XMAX(J)                              F600 970
      SMUL2=AMIN1(SCAL(1),SCAL(2),SCAL(3),SCAL(4))                     F600 980
      GO TO 780                                                        F600 990
C     ***** AUTOMATIC SCALE AND POSITION *****                         F6001000
  755 DO 760 J=1,2                                                     F6001010
  760 SCAL(J)=(XLNG(J)-BRDR*2.)/(XMAX(J)-XMIN(J))                      F6001020
      SMUL2=AMIN1(SCAL(1),SCAL(2))                                     F6001030
C     ***** AUTOMATIC POSITION *****                                   F6001040
  765 DO 770 J=1,2                                                     F6001050
  770 XO(J)=.5*(XLNG(J)-SMUL2*(XMAX(J)+XMIN(J)))                       F6001060
  780 SMULT=SMULT*SMUL2                                                F6001070
      VIEW=VIEW*SMUL2                                                  F6001080
  785 SCAL1=SCAL1*SMULT                                                F6001090
  790 SCL=SCAL1*SCAL2                                                  F6001100
C     ***** ELIMINATE ALL PREVIOUSLY STORED OVERLAP INFORMATION *****  F6001110
      CALL LAP500(0)                                                   F6001120
      RETURN                                                           F6001130
      END                                                              F6001140


      SUBROUTINE F700                                                  F700  10
C     ***** SUBROUTINE TO DRAW ELLIPSOIDS *****                        F700  20
      DIMENSION EYE(3),VIEWV(3),X(3),Z(3)                              F700  30
      REAL*8 CHEM                                                      F700  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)   F700  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)F700  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)F700  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)F700  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)  F700  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)  F700 100
      DIMENSION XLNG(3),XO(3),XT(3)                                    F700 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  F700 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F700 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F700 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2  F700 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                               F700 160
C     ***** SET ELLIPSOID GRAPHIC DETAILS *****                        F700 170
      ITILT=0                                                          F700 180
      NG=0                                                             F700 190
      NFIRST=1                                                         F700 200
      NPLANE=AIN(1)                                                    F700 210
      IF(NPLANE-1)720,715,720                                          F700 220
  715 NFIRST=4                                                         F700 230
      NPLANE=4                                                         F700 240
  720 NSOLID=AIN(2)                                                    F700 250
      NDOT=64/2**( IABS(NSOLID))                                       F700 260
      LINES=AIN(3)                                                     F700 270
      NDASH=AIN(4)                                                     F700 280
      CHSYM=AIN(5)                                                     F700 290
      DH=AIN(6)-CHSYM*17./7.                                           F700 300
      DV=AIN(7)-CHSYM*.5                                               F700 310
C     ***** ESTABLISH REFERENCE POINT OF VIEW *****                    F700 320
      T1=1.E6                                                          F700 330
      IF(VIEW) 740,740,735                                             F700 340
  735 T1=VIEW/SCAL1                                                    F700 350
  740 DO 741 J=1,3                                                     F700 360
  741 EYE(J)=REFV(J,3)*T1+ORGN(J)                                      F700 370
       LNS=-1                                                          F700 380
C     ***** LOOP THROUGH ATOM LIST *****                               F700 390
      DO 1105 ITOM=1,LATM                                              F700 400
      T1=ATOMS(1,ITOM)                                                 F700 410
      IF(AIN(10))744,744,742                                           F700 420
  742 T2=AINT(T1/100000.)                                              F700 430
      IF(T2-AIN(10))1105,743,743                                       F700 440
  743 IF(AIN(11)-T2)1105,744,744                                       F700 450
  744 CALL XYZ(T1,X,2)                                                 F700 460
      IF(NG) 758,746,758                                               F700 470
  746 CALL PLTXY(X,Z)                                                  F700 480
      K=T1/100000.                                                     F700 490
      L=T1-FLOAT (K)*100000.                                           F700 500
      IF(NJ2-10) 747,754,754                                           F700 510
  747 LNS=MOD(LNS+1,18)                                                F700 520
      IF(LNS) 749,748,749                                              F700 530
  748 WRITE (NOUT,751) (TITLE(I),I=1,18)                               F700 540
      WRITE (NOUT,752)                                                 F700 550
  749 WRITE (NOUT,750)CHEM(K),K,L,Z(1),Z(2),(X(I),I=1,3),(XT(          F700 560
     1I),I=1,3)                                                        F700 570
  750 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)    2F8.2,3X,3F8.3,11X,3F8.4)  F700 580
  751 FORMAT(1H110X,18A4)                                              F700 590
  752 FORMAT(1H010X,18HSYMBOL   ATOM CODE7X,16HPLOTTER X,Y(IN.) 3X,21HCAF700 600
     1RTESIAN X,Y,Z (IN.)15X,20HCRYSTAL SYSTEM X,Y,Z/1H 19X,45H(DIRECTIOF700 610
     2N COSINES(I,J),I=1,3),RMSD(J)),J=1,312X,42HFOR PRINCIPAL AXES BASEF700 620
     3D ON WORKING SYSTEM/1H )                                         F700 630
  754 IF(EDGE-BRDR*.75)755,760,760                                     F700 640
  755 NG=10                                                            F700 650
  758 CALL ERPNT(T1,700)                                               F700 660
      GO TO 1105                                                       F700 670
C     ***** CALL OVERLAP ROUTINE *****                                 F700 680
  760 ICQ=0                                                            F700 690
      CALL LAP700(ITOM,ICQ)                                            F700 700
      IF(ICQ) 762,764,764                                              F700 710
C     ***** OMIT HIDDEN ATOM *****                                     F700 720
  762 NG=14                                                            F700 730
      GO TO 758                                                        F700 740
  764 IF(CHSYM) 775,775,765                                            F700 750
C     ***** PLOT CHEMICAL SYMBOLS *****                                F700 760
  765 T4=1.                                                            F700 770
      IF(VIEW) 767,767,766                                             F700 780
  766 T4=VIEW/(VIEW-X(3))                                              F700 790
  767 T3=CHSYM*T4                                                      F700 800
      T4=DISP*T4*.5                                                    F700 810
      V1(1)=X(1)+DH*SYMB(1,1)+DV*SYMB(1,2)                             F700 820
      V1(2)=X(2)+DH*SYMB(2,1)+DV*SYMB(2,2)                             F700 830
      V1(3)=X(3)                                                       F700 840
      CALL PLTXY(V1,V3)                                                F700 850
      IF(EDGE-CHSYM) 775,768,768                                       F700 860
  768 V2(3)=0.                                                         F700 870
      DO 770 I=1,3,2                                                   F700 880
      V2(1)=V3(1)+FLOAT(I-2)*T4                                        F700 890
      DO 770 J=1,3,2                                                   F700 900
      V2(2)=V3(2)+FLOAT(J-2)*T4                                        F700 910
      CALL SIMBOL(V2(1),V2(2),T3,CHEM(K),THETA,6)                      F700 920
      IF(T4) 775,775,770                                               F700 930
  770 CONTINUE                                                         F700 940
  775 IF(NPLANE) 1105,1105,780                                         F700 950
C     ***** ELLIPSOID PRINC VECTORS TOWARD VIEWER *****                F700 960
  780 CALL PAXES(T1,2)                                                 F700 970
      IF(NG) 758,783,758                                               F700 980
  783 CALL DIFV(EYE,XT,VIEWV)                                          F700 990
      CALL UNIT(VIEWV,VIEWV,-1)                                        F7001000
      CALL VM(VIEWV,AA,V2)                                             F7001010
      DO 795 I=1,3                                                     F7001020
      IF(VV(V2,PAT(1,I)))785,795,795                                   F7001030
  785 DO 790 J=1,3                                                     F7001040
      PAC(J,I)=-PAC(J,I)                                               F7001050
  790 PAT(J,I)=-PAT(J,I)                                               F7001060
  795 CONTINUE                                                         F7001070
      DO 800 J=1,3                                                     F7001080
      PAC(J,4)=PAC(J,1)                                                F7001090
  800 PAC(J,5)=PAC(J,2)                                                F7001100
      IF(NJ2-10) 802,803,803                                           F7001110
  801 FORMAT(1H 13X,3(3X,3F8.4,F8.5)/1H )                              F7001120
  802 WRITE (NOUT,801) ((PAC(J,K),J=1,3),RMS(K) ,K=1,3)                F7001130
C     ***** V4 = VECTOR NORMAL TO POLAR PLANE *****                    F7001140
  803 CALL VM(VIEWV,AAWRK,V6)                                          F7001150
      CALL UNIT(V6,V6,1)                                               F7001160
      CALL MV(Q,V6,V4)                                                 F7001170
      CALL UNIT(V4,V4,1)                                               F7001180
C     ***** SET PLOTTING RESOLUTION FOR ELLIPSOID *****                F7001190
      T3=RMS(3)*SCL                                                    F7001200
      NRESOL=1                                                         F7001210
      NBIS=5                                                           F7001220
      DO 805 J=1,3                                                     F7001230
      IF(T3-RES(J)) 804,810,810                                        F7001240
  804 NBIS=NBIS-1                                                      F7001250
  805 NRESOL=NRESOL*2                                                  F7001260
  810 NRES1=NRESOL+1                                                   F7001270
C     ***** LOOP THROUGH PRINC AND POLAR PLANES *****                  F7001280
      DO 1100 II=NFIRST,NPLANE                                         F7001290
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      II0=MOD(II+2,3)+1                                                 F7001300
      II1=MOD(II,3)+1                                                   F7001310
      II2=MOD(II+1,3)+1                                                 F7001320
C     ***** GENERATE CONJUGATE DIAMETERS *****                          F7001330
      IF(.99938- ABS(VV(V4,PAC(1,II2))))820,820,830                     F7001340
  820 T1=RMS(II0)*SCL                                                   F7001350
      T2=RMS(II1)*SCL                                                   F7001360
      DO 825 J=1,3                                                      F7001370
      DA(J,1)=PAC(J,II0)*T1                                             F7001380
  825 DA(J,2)=PAC(J,II1)*T2                                             F7001390
      GO TO 850                                                         F7001400
  830 CALL NORM(PAC(1,II0),PAC(1,II1),V1,1)                             F7001410
      CALL NORM(V1,V4,V2,1)                                             F7001420
      CALL UNIT(V2,V2,1)                                                F7001430
      CALL MV(Q,V2,V3)                                                  F7001440
      IF(II-4) 835,840,840                                              F7001450
  835 CALL NORM(V3,V1,V5,1)                                             F7001460
      GO TO 843                                                         F7001470
  840 CALL NORM(V3,V4,V5,1)                                             F7001480
  843 CALL UNIT(V5,V5,1)                                                F7001490
      T1=SCL/SQRT(VMV(V2,Q,V2))                                         F7001500
      T2=SCL/SQRT(VMV(V5,Q,V5))                                         F7001510
      DO 845 J=1,3                                                      F7001520
      DA(J,1)=V2(J)*T1                                                  F7001530
  845 DA(J,2)=V5(J)*T2                                                  F7001540
C     ***** GENERATE ELLIPSE *****                                      F7001550
  850 CALL RADIAL(NBIS)                                                 F7001560
      IF(II-4) 900,851,851                                              F7001570
  851 IF(NSOLID) 859,859,852                                            F7001580
C     ***** PLOT DOTTED BOUNDARY ELLIPSE *****                          F7001590
  852 IF(NDOT-NRESOL) 853,855,855                                       F7001600
  853 CALL RADIAL(NSOLID-1)                                             F7001610
  855 CALL PROJ(D,DP,X,XO,VIEW,1,129,NDOT)                              F7001620
      DO 857 J=1,129,NDOT                                               F7001630
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    F7001640
      DO 856 I=1,3,2                                                    F7001650
      T1=FLOAT(I-2)*DISP                                                F7001660
      DO 856 K=1,3,2                                                    F7001670
      T2=FLOAT(K-2)*DISP                                                F7001680
      CALL DRAW(DP(1,J),T1,T2,2)                                        F7001690
      IF(DISP) 857,857,856                                              F7001700
  856 CONTINUE                                                          F7001710
  857 CONTINUE                                                          F7001720
      GO TO 1100                                                        F7001730
C     ***** PLOT SOLID BOUNDARY ELLIPSE *****                           F7001740
  859 CALL PROJ(D,DP,X,XO,VIEW,1,129,NRESOL)                            F7001750
      CALL DRAW(DP,0.,0.,3)                                             F7001760
      DO 860 J=NRES1,129,NRESOL                                         F7001770
  860 CALL DRAW(DP(1,J),0.,0.,2)                                        F7001780
      IF(DISP) 1100,1100,865                                            F7001790
C     ***** BOUNDARY ANNULUS AS A LINEAR FUNCTION OF HEIGHT *****       F7001800
  865 CALL DIFV(XT,ORGN,V1)                                             F7001810
      T5=VV(V1,AAREV(1,3))*SCAL1                                        F7001820
      NCYCLE=.5+(AIN(8)+T5*AIN(9))/DISP                                 F7001830
      IF(NCYCLE) 1100,1100,870                                          F7001840
  870 T3=(2.*DISP)/(T1+T2)                                              F7001850
C     ***** INCREASE ANNULAR THICKNESS *****                            F7001860
      DO 875 I=1,NCYCLE                                                 F7001870
      T4=T3*FLOAT(I)                                                    F7001880
      DO 875 J=1,129,NRESOL                                             F7001890
  875 CALL DRAW(DP(1,J),D(1,J)*T4,D(2,J)*T4,2)                          F7001900
      GO TO 1100                                                        F7001910
  900 CALL PROJ(D,DP,X,XO,VIEW,1,65,NRESOL)                             F7001920
C     ***** PLOT HALF AN ELLIPSE *****                                  F7001930
      CALL DRAW(DP,0.,0.,3)                                             F7001940
      DO 905 J=NRES1,65,NRESOL                                          F7001950
  905 CALL DRAW(DP(1,J),0.,0.,2)                                        F7001960
      IF(DISP) 930,930,910                                              F7001970
C     ***** ACCENTUATE FRONT HALF *****                                 F7001980
  910 DO 925 I=1,3,2                                                    F7001990
      T2=FLOAT(I-2)*DISP                                                F7002000
      DO 915 J=1,65,NRESOL                                              F7002010
      K=66-J                                                            F7002020
  915 CALL DRAW(DP(1,K),DISP,T2,2)                                      F7002030
      DO 925 K=1,65,NRESOL                                              F7002040
  925 CALL DRAW(DP(1,K),-DISP,-T2,2)                                    F7002050
  930 IF(NSOLID) 940,967,935                                            F7002060
  935 L=NDOT                                                            F7002070
      IF(NDOT-NRESOL) 938,945,940                                       F7002080
  938 CALL RADIAL(NSOLID-1)                                             F7002090
      GO TO 945                                                         F7002100
  940 L=NRESOL                                                          F7002110
  945 CALL PROJ(D(1,65),DP(1,65),X,XO,VIEW,1,65,L)                      F7002120
      IF(NSOLID) 960,967,950                                            F7002130
C     ***** DOTTED LINE ON REVERSE SIDE *****                           F7002140
  950 DO 958 J=65,129,NDOT                                              F7002150
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    F7002160
      DO 955 I=1,3,2                                                    F7002170
      T1=FLOAT(I-2)*DISP                                                F7002180
      DO 955 K=1,3,2                                                    F7002190
      T2=FLOAT(K-2)*DISP                                                F7002200
      CALL DRAW(DP(1,J),T1,T2,2)                                        F7002210
      IF(DISP) 958,958,955                                              F7002220
  955 CONTINUE                                                          F7002230
  958 CONTINUE                                                          F7002240
      GO TO 967                                                         F7002250
C     ***** SINGLE LINE ON REVERSE SIDE *****                           F7002260
  960 DO 965 J=65,129,NRESOL                                            F7002270
  965 CALL DRAW(DP(1,J),0.,0.,2)                                        F7002280
C     ***** DETAIL INTERIOR FEATURES *****                              F7002290
  967 T2=NDASH*2                                                        F7002300
      DO 975 J=1,3                                                      F7002310
      T1=PAC(J,II0)*RMS(II0)*SCL                                        F7002320
      DA(J,1)=T1                                                        F7002330
      DA(J,2)=PAC(J,II1)*RMS(II1)*SCL                                   F7002340
      DA(J,3)=0.                                                        F7002350
      IF(NDASH) 975,975,970                                             F7002360
  970 V1(J)=-T1                                                         F7002370
      V2(J)=T1/T2                                                       F7002380
  975 CONTINUE                                                          F7002390
      IF(NDASH) 987,987,980                                             F7002400
C     ***** DASHED LINE FOR REVERSE AXIS *****                          F7002410
  980 DO 985 J=1,NDASH                                                  F7002420
      DO 985 K=1,2                                                      F7002430
      L=4-K                                                             F7002440
      CALL PROJ(V1,DP,X,XO,VIEW,1,1,1)                                  F7002450
      CALL DRAW(DP,0.,0.,L)                                             F7002460
      DO 985 I=1,3                                                      F7002470
  985 V1(I)=V1(I)+V2(I)                                                 F7002480
C     ***** SOLID LINE FOR FORWARD AXIS *****                           F7002490
  987 IF(LINES) 1100,1100,988                                           F7002500
  988 CALL PROJ(DA,DP,X,XO,VIEW,1,3,1)                                  F7002510
      T1=DISP*.5                                                        F7002520
      DO 990 I=1,3,2                                                    F7002530
      T2=FLOAT(2-I)*T1                                                  F7002540
      CALL DRAW(DP,T1,T2,3)                                             F7002550
      CALL DRAW(DP(1,3),T1,T2,2)                                        F7002560
      IF(DISP) 1000,1000,989                                            F7002570
  989 CALL DRAW(DP(1,3),-T1,T2,2)                                       F7002580
  990 CALL DRAW(DP,-T1,T2,2)                                            F7002590
C     ***** SHADE QUADRANT BETWEEN TWO PRINCIPAL AXES *****             F7002600
 1000 L=LINES-1                                                         F7002610
      IF(L) 1100,1100,1005                                              F7002620
 1005 T2=LINES                                                          F7002630
      DO 1025 I=1,L                                                     F7002640
      T1=FLOAT(I)/T2                                                    F7002650
      T3=SQRT(1.-T1*T1)                                                 F7002660
      IF(MOD(I,2)) 1010,1015,1010                                       F7002670
 1010 M=I*2                                                             F7002680
      N=M-1                                                             F7002690
      GO TO 1020                                                        F7002700
 1015 N=I*2                                                             F7002710
      M=N-1                                                             F7002720
 1020 DO 1025 J=1,3                                                     F7002730
      T4=DA(J,1)*T1                                                     F7002740
      D(J,M)=T4                                                         F7002750
 1025 D(J,N)=DA(J,2)*T3+T4                                              F7002760
      L=L*2                                                             F7002770
      CALL PROJ(D,DP,X,XO,VIEW,1,L,1)                                   F7002780
      DO 1030 I=2,L,2                                                   F7002790
      CALL DRAW(DP(1,I-1),0.,0.,3)                                      F7002800
 1030 CALL DRAW(DP(1,I),0.,0.,2)                                        F7002810
 1100 CONTINUE                                                          F7002820
 1105 CONTINUE                                                          F7002830
C     ***** ELIMINATE LOCAL OVERLAP INFORMATION BEFORE RETURNING *****  F7002840
      CALL LAP500(-1)                                                   F7002850
      RETURN                                                            F7002860
      END                                                               F7002870


      SUBROUTINE F800                                                   F800  10
C     ***** SUBROUTINE FINDS ATOM PAIRS FOR BONDS *****                 F800  20
      DIMENSION IA(3),W1(6)                                             F800  30
      REAL*8 CHEM                                                       F800  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F800  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F800  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F800  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAI(3,3),Q(3,3),REFV(3,3) F800  80
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      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F800  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F800 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F800 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F800 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F800 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F800 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F800 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F800 160
      LNS=-4                                                            F800 170
      IF(MOD(NJ2,10)-2) 805,848,848                                     F800 180
C     ***** EXPLICIT DESCRIPTION *****                                  F800 190
  805 II=0                                                              F800 200
      IF(NCD) 810,810,815                                               F800 210
  810 NG=11                                                             F800 220
      CALL ERPNT(0.,NJ*100+NJ2)                                         F800 230
      GO TO 980                                                         F800 240
  815 II=II+1                                                           F800 250
      IF(140-II) 980,980,820                                            F800 260
  820 T1=AIN(II)                                                        F800 270
      IF(T1) 815,815,825                                                F800 280
  825 II=II+1                                                           F800 290
      T2=AIN(II)                                                        F800 300
      IF(T2) 815,815,830                                                F800 310
  830 IF(NJ2-10) 832,838,838                                            F800 320
  832 LNS=MOD(LNS+4,56)                                                 F800 330
      IF(LNS) 838,834,838                                               F800 340
  834 WRITE (NOUT,835) (TITLE(I),I=1,18)                                F800 350
  835 FORMAT(1H110X,18A4)                                               F800 360
      WRITE (NOUT,837)                                                  F800 370
  837 FORMAT(1H010X,18HSYMBOL   ATCM CODE6X,16HPLOTTER X,Y(IN.) 6X,21HCAF800 380
     1RTESIAN X,Y,Z (IN.) 17X,20HCRYSTAL SYSTEM X,Y,Z/1H )              F800 390
C     ***** CHECK IF BOND ATOMS ARE IN ATOMS LIST (FOR OVERLAP CALC) ***F800 400
  838 NA1=0                                                             F800 410
      NA2=0                                                             F800 420
      IF(LATM-2) 845,839,839                                            F800 430
  839 N2=2                                                              F800 440
      DO 844 K=1,LATM                                                   F800 450
      T3=ATOMS(1,K)                                                     F800 460
      IF(T3-T1) 841,840,841                                             F800 470
  840 NA1=K                                                             F800 480
      GO TO 843                                                         F800 490
  841 IF(T3-T2) 844,842,844                                             F800 500
  842 NA2=K                                                             F800 510
  843 N2=N2-1                                                           F800 520
      IF(N2) 845,845,844                                                F800 530
  844 CONTINUE                                                          F800 540
  845 IF(NA2-NA1) 846,847,847                                           F800 550
  846 NA3=NA1                                                           F800 560
      NA1=NA2                                                           F800 570
      NA2=NA3                                                           F800 580
      T3=T1                                                             F800 590
      T1=T2                                                             F800 600
      T2=T3                                                             F800 610
  847 CALL BOND(T1,T2,1,NA1,NA2)                                        F800 620
      GO TO 815                                                         F800 630
C     ***** IMPLICIT DESCRIPTION *****                                  F800 640
  848 IF(LATM-2) 810,850,850                                            F800 650
  850 SCAL3=SCAL1                                                       F800 660
      SCAL1=1.                                                          F800 670
      DO 855 I=1,LATM                                                   F800 680
  855 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                 F800 690
      SCAL1=SCAL3                                                       F800 700
      IF(NCD) 810,810,860                                               F800 710
  860 WRITE (NOUT,861)                                                  F800 720
  861 FORMAT(1H010X,20HBOND SELECTION CODES//11X,94H(SEQUENCE(A)) (SEQUENF800 730
     1CE(B)) (BOND) (DISTANCES) ( BOND ) (PERSP.--LABELS) (NORMAL--LABELS) (F800 740
     2DIGITS) /11X,93H(  MIN   MAX )(  MIN   MAX ) (TYPE) (MIN    MAX) (RADIF800 750
     3US) (HEIGHT  OFFSET) (HEIGHT  OFFSET) (NUMBER))                   F800 760
      DMAX=0.                                                           F800 770
      DO 870 I=1,NCD                                                    F800 780
      IF(DMAX-CD(2,I)) 865,870,870                                      F800 790
  865 DMAX=CD(2,I)                                                      F800 800
  870 WRITE (NOUT,871) (KD(J,I),J=1,5),(CD(J,I),J=1,8)                  F800 810
  871 FORMAT(1H 10XI6,I5,I8,I5,I8,2F6.2,5F8.3,F7.0)                     F800 820
      DMAX=DMAX*DMAX                                                    F800 830
C     ***** LOOP THROUGH ATOMS ARRAY *****                              F800 840
      DO 977 M=1,LATM                                                   F800 850
      NA1=M                                                             F800 860
      T1=ATOMS(1,M)                                                     F800 870
      IA(1)=T1/100000.                                                  F800 880
      IA(3)=IA(1)                                                       F800 890
      W1(1)=ATOMS(2,M)                                                  F800 900
      W1(2)=ATOMS(3,M)                                                  F800 910
      W1(3)=ATOMS(4,M)                                                  F800 920
      L=M+1                                                             F800 930
      IF(LATM-L) 977,872,872                                            F800 940
  872 DO 975 N=L,LATM                                                   F800 950
      NA2=N                                                             F800 960
      DIST=(ATOMS(2,N)-W1(1))**2                                        F800 970
      IF(DMAX-DIST) 975,873,873                                         F800 980
  873 DIST=DIST+(ATOMS(3,N)-W1(2))**2                                   F800 990
      IF(DMAX-DIST) 975,874,874                                         F8001000
  874 DIST=DIST+(ATOMS(4,N)-W1(3))**2                                   F8001010
      IF(DMAX-DIST) 975,875,875                                         F8001020
  875 DIST=SQRT(DIST)                                                   F8001030
      T2=ATOMS(1,N)                                                     F8001040
      IA(2)=T2/100000.                                                  F8001050
C     ***** SELECT BONDS ACCORDING TO CODES *****                       F8001060
      DO 950 J=1,NCD                                                    F8001070
      JB=J                                                              F8001080
      IF(DIST-CD(1,J))    950,880,880                                   F8001090
  880 IF(CD(2,J)-DIST)    950,881,881                                   F8001100
  881 DO 885 K=1,2                                                      F8001110
      IF(IA(K)-KD(1,J))   885,882,882                                   F8001120
  882 IF(KD(2,J)-IA(K))   885,883,883                                   F8001130
  883 IF(IA(K+1)-KD(3,J)) 885,884,884                                   F8001140
  884 IF(KD(4,J)-IA(K+1)) 885,890,890                                   F8001150
  885 CONTINUE                                                          F8001160
      GO TO 950                                                         F8001170
C     ***** CHECK FOR POLYHEDRA CODE *****                              F8001180
  890 IF(CD(4,J)) 900,955,955                                           F8001190
  900 W1(4)=ATOMS(2,N)                                                  F8001200
      W1(5)=ATOMS(3,N)                                                  F8001210
      W1(6)=ATOMS(4,N)                                                  F8001220
      KM1=ABS(CD(4,J))                                                  F8001230
      KM2=ABS(CD(5,J))                                                  F8001240
      DSQ1=(CD(6,J))**2                                                 F8001250
      DSQ2=(CD(7,J))**2                                                 F8001260
C     ***** SEARCH FOR POLYHEDRA CENTER *****                           F8001270
      DO 935 IM=1,LATM                                                  F8001280
      K3=ATOMS(1,IM)/100000.                                            F8001290
      IF(K3-KM1) 935,905,905                                            F8001300
  905 IF(KM2-K3) 935,910,910                                            F8001310
C     ***** CHECK POLYHEDRA DISTANCE RANGE *****                        F8001320
  910 DO 930 J1=1,4,3                                                   F8001330
      DSQ=(ATOMS(2,IM)-W1(J1))**2                                       F8001340
      IF(DSQ2-DSQ) 935,915,915                                          F8001350
  915 DSQ=DSQ+(ATOMS(3,IM)-W1(J1+1))**2                                 F8001360
      IF(DSQ2-DSQ) 935,920,920                                          F8001370
  920 DSQ=DSQ+(ATOMS(4,IM)-W1(J1+2))**2                                 F8001380
      IF(DSQ2-DSQ) 935,925,925                                          F8001390
  925 IF(DSQ-DSQ1) 935,930,930                                          F8001400
  930 CONTINUE                                                          F8001410
      GO TO 955                                                         F8001420
  935 CONTINUE                                                          F8001430
C     ***** END OF POLYHEDRA CHECK *****                                F8001440
  950 CONTINUE                                                          F8001450
      GO TO 975                                                         F8001460
C     ***** PREPARE TO DRAW BOND *****                                  F8001470
  955 IF(NJ2-10) 960,970,970                                            F8001480
  960 LNS=MOD(LNS+4,56)                                                 F8001490
      IF(LNS) 965,965,970                                               F8001500
  965 WRITE (NOUT,835) (TITLE(I),I=1,18)                                F8001510
      WRITE (NOUT,837)                                                  F8001520
  970 CALL BOND(T1,T2,JB,NA1,NA2)                                       F8001530
  975 CONTINUE                                                          F8001540
  977 CONTINUE                                                          F8001550
C     ***** ELIMINATE LOCAL OVERLAP INFORMATION BEFORE RETURNING *****  F8001560
  980 IF(NJ2-21) 985,990,990                                            F8001570
  985 CALL LAP500(-1)                                                   F8001580
  990 RETURN                                                            F8001590
      END                                                               F8001600


      SUBROUTINE F900                                                   F900  10
      DIMENSION X(3),XW(3,5),Y(3),Z(3)                                  F900  20
      REAL*8 CHEM                                                       F900  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F900  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)F900  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F900  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F900  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F900  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F900  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     F900 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F900 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F900 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F900 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F900 140
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      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F900 150
C     ***** LABELING FUNCTION SUBROUTINE *****                          F900 160
      ITILT=0                                                           F900 170
      NJ3=MOD(NJ2,10)                                                   F900 180
      TH=THETA                                                          F900 190
      SINTH=SYMB(2,1)                                                   F900 200
      COSTH=SYMB(1,1)                                                   F900 210
      ILAST=1                                                           F900 220
      IF(AIN(2)-11100.)910,910,905                                      F900 230
  905 ILAST=2                                                           F900 240
  910 DO 925 II=1,ILAST                                                 F900 250
C     ***** OBTAIN WORKING CARTESIAN COORDINATES *****                  F900 260
      CALL XYZ(AIN(II),XW(1,II),2)                                      F900 270
      IF(NG)915,925,915                                                 F900 280
  912 NG=15                                                             F900 290
  915 CALL ERPNT(AIN(II),NJ*100+NJ2)                                    F900 300
      GO TO 1199                                                        F900 310
  925 CALL XYZ(AIN(II),XW(1,II+3),3)                                    F900 320
      II=1                                                              F900 330
C     ***** FIND MEAN REFERENCE POINT *****                             F900 340
      DO 930 J=1,3                                                      F900 350
      T2=XW(J,ILAST)                                                    F900 360
      T1=XW(J,1)                                                        F900 370
      XW(J,3)=T2-T1                                                     F900 380
  930 X(J)=(T2+T1)*.5                                                   F900 390
C     ***** PERSPECTIVE SCALING FACTOR *****                            F900 400
      SCAL=1.                                                           F900 410
      IF(VIEW)940,940,935                                               F900 420
  935 SCAL=VIEW/(VIEW-X(3))                                             F900 430
  940 HGT=SCAL*AIN(5)                                                   F900 440
      IF(NJ2-3)960,950,945                                              F900 450
  945 IF(NJ2-6)950,950,960                                              F900 460
C     ***** PROJECTED VECTOR BASELINE *****                             F900 470
  950 CALL PLTXY(XW(1,4),V1)                                            F900 480
      CALL PLTXY(XW(1,5),V2)                                            F900 490
      T1=V2(1)-V1(1)                                                    F900 500
      T2=V2(2)-V1(2)                                                    F900 510
      T3=SQRT(T1*T1+T2*T2)                                              F900 520
      IF(T3)912,912,955                                                 F900 530
  955 COSTH=T1/T3                                                       F900 540
      SINTH=T2/T3                                                       F900 550
      TH=ARCCOS(COSTH)                                                  F900 560
      IF(SINTH)958,960,960                                              F900 570
  958 TH=-TH                                                            F900 580
  960 IF(NJ2-13)965,985,985                                             F900 590
C     ***** FIND CENTER OF PROJECTED LABEL *****                        F900 600
  965 Y(1)=SCAL*(X(1)+AIN(6)*COSTH-AIN(7)*SINTH)+XO(1)                  F900 610
      Y(2)=SCAL*(X(2)+AIN(6)*SINTH+AIN(7)*COSTH)+XO(2)                  F900 620
      Y(3)=0.                                                           F900 630
C     ***** CHECK FOR LEGEND RESET *****                                F900 640
      DO 980 J=1,2                                                      F900 650
      T1=AIN(J+2)                                                       F900 660
      IF(T1)975,980,970                                                 F900 670
  970 Y(J)=T1                                                           F900 680
      GO TO 980                                                         F900 690
  975 Y(J)=XLNG(J)+T1                                                   F900 700
  980 CONTINUE                                                          F900 710
C     ***** SET PARAMETERS FOR INDIVIDUAL FUNCTIONS *****               F900 720
  985 GO TO(990,995,995,1000,1000,1000,915,1105,1105,915,915,915,1005,10F900 730
     105,1005,1005,915),NJ2                                             F900 740
  990 T6=17.                                                            F900 750
      L=AIN(1)/100000.                                                  F900 760
      ILAST=1                                                           F900 770
      DXW=0.                                                            F900 780
      DYW=0.                                                            F900 790
      GO TO 1030                                                        F900 800
  995 T6=215.                                                           F900 810
      ILAST=18                                                          F900 820
      T1=HGT*24./7.                                                     F900 830
      DXW=COSTH*T1                                                      F900 840
      DYW=SINTH*T1                                                      F900 850
      GO TO 1030                                                        F900 860
 1000 T6=10+3*(NJ3-4)                                                   F900 870
      DIST=SQRT(VV(XW(1,3),XW(1,3)))/SCAL1                              F900 880
      GO TO 1030                                                        F900 890
C     ***** TRUE PERSPECTIVE LABELS *****                               F900 900
 1005 CALL UNIT(XW(1,3),VT(1,1),1)                                      F900 910
      IF(ABS(VT(3,1))-.9994)1010,912,912                                F900 920
C     ***** FORM PERSPECTIVE ROTATION MATRIX *****                      F900 930
 1010 CALL NORM(AID(1,3),VT(1,1),VT(1,2),1)                             F900 940
      CALL UNIT(VT(1,2),VT(1,2),1)                                      F900 950
      CALL NORM(VT(1,1),VT(1,2),VT(1,3),1)                              F900 960
      DO 1015 J=1,3                                                     F900 970
 1015 VT(J,4)=X(J)                                                      F900 980
      ITILT=1                                                           F900 990
      HGT=AIN(5)                                                        F9001000
      TH=0.                                                             F9001010
      Y(3)=X(3)                                                         F9001020
      Y(2)=X(2)+AIN(7)-HGT*.5                                           F9001030
      IF(NJ2-13)1030,1025,1020                                          F9001040
C     ***** PERSPECTIVE BOND LABELS *****                               F9001050
 1020 Y(1)=X(1)+AIN(6)-HGT*FLOAT(22+3*(6-NJ3))/7.                       F9001060
      DIST=SQRT(VV(XW(1,3),XW(1,3)))/SCAL1                              F9001070
      GO TO 1050                                                        F9001080
C     ***** PERSPECTIVE TITLES *****                                    F9001090
 1025 Y(1)=X(1)+AIN(6)-HGT*215./7.                                      F9001100
      ILAST=18                                                          F9001110
      DXW=HGT*24./7.                                                    F9001120
      DYW=0.                                                            F9001130
      GO TO 1050                                                        F9001140
 1030 DH=HGT*T6/7.                                                      F9001150
      DV=HGT*.5                                                         F9001160
      Y(1)=Y(1)-DH*COSTH+DV*SINTH                                       F9001170
      Y(2)=Y(2)-DH*SINTH-DV*COSTH                                       F9001180
      Y(3)=0.                                                           F9001190
C     ***** PLOT VARIOUS LABELS *****                                   F9001200
 1050 Z(3)=Y(3)                                                         F9001210
      XO(3)=Y(3)                                                        F9001220
      GO TO(1060,1060,1060,1090,1090,1090,915,1105,1105),NJ3            F9001230
 1060 DO 1085 I=1,ILAST                                                 F9001240
      DO 1075 J=1,3,2                                                   F9001250
      Z(1)=Y(1)+FLOAT(J-2)*DISP*.5                                      F9001260
      DO 1075 K=1,3,2                                                   F9001270
      Z(2)=Y(2)+FLOAT(K-2)*DISP*.5                                      F9001280
      IF(NJ3-2)1065,1068,1068                                           F9001290
C     ***** PLOT CHEMICAL SYMBOL *****                                  F9001300
 1065 CALL SIMBOL(Z(1),Z(2),HGT,CHEM(L),TH,6)                           F9001310
      GO TO 1070                                                        F9001320
C     ***** PLOT TITLES *****                                           F9001330
 1068 CALL SIMBOL(Z(1),Z(2),HGT,TITLE2(I),TH,4)                         F9001340
 1070 IF(DISP)1080,1080,1075                                            F9001350
 1075 CONTINUE                                                          F9001360
 1080 Y(1)=Y(1)+DXW                                                     F9001370
 1085 Y(2)=Y(2)+DYW                                                     F9001380
      GO TO 1199                                                        F9001390
C     ***** PLOT BOND DISTANCE LABELS *****                             F9001400
 1090 I9=NJ3-3                                                          F9001410
      T9=10.**I9                                                        F9001420
      DISTR=AINT((DIST*T9)+0.5)/T9 +.0001                               F9001430
      CALL NUMBUF(Y(1),Y(2),HGT,DISTR,TH,I9)                            F9001440
      GO TO 1199                                                        F9001450
C     ***** PLOT CENTERED SYMBOLS *****                                 F9001460
 1105 CALL SIMBOL(Y(1),Y(2),HGT, IFIX(AIN(8)),TH,7-NJ3)                 F9001470
 1199 ITILT=0                                                           F9001480
      RETURN                                                            F9001490
      END                                                               F9001500


      SUBROUTINE F1000                                                  F100  10
      DIMENSION D6(3,3),D15(15),D6L(3,3),DQ(6),QQ(6)                    F100  20
      DIMENSION C1(3),QF(3,3),C3(10),CE(10)                             F100  30
      DIMENSION CIJK(3,3,3),GAMMA(3,3,3),B2(3,3),B3(3,3)                F100  40
      DIMENSION Z0(3),Z1(3),Z2(3),DZ0(3),DZ1(3),LINE(22,2),HEAD(22)     F100  50
      REAL*8 CHEM                                                       F100  60
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F100  70
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F100  80
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F100  90
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F100 100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F100 110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F100 120
      DIMENSION XLNG(3),XO(3),XT(3)                                     F100 130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F100 140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD F100 150
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F100 160
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F100 170
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F100 180
      EQUIVALENCE(LINE(1),HEAD(1))                                      F100 190
C**** SUBROUTINE TO ANALYZE TENSORS OF HIGHER CUMULANTS ****            F100 200
C     COLUMN  6- 9  = 1000                                              F100 210
C     COLUMN 10-18 FIRST ATOM WITH SKEW TENSOR, IF 0 OR BLANK IS SET = 1F100 220
C     COLUMN 19-27 LAST ATOM WITH SKEW TENSOR, IF ZERO IS SET = NATOM   F100 230
C     COLUMN 28-36 IF ZERO SHIFT POSITION PARAMETERS OF ATOM TO MODE    F100 240
C                  IF .GT. ZERO, DO NOT SHIFT TO MODE                   F100 250
C     COLUMN 37-45 PSI AND CHI IF ZERO, ONLY PSI IF +, ONLY CHI IF MINUSF100 260
C**** CONTINUATION CARD IF A 1 IN COLUMN 3 OF PREVIOUS CARD ****        F100 270
C     COLUMN 10-18 SCALE FACTOR FOR MAPS, IF ZERO, NO MAPS              F100 280
C     COLUMN 19-27 NUMBER OF GRID POINTS ALONG X IN MAP                 F100 290
C     COLUMN 28-36                                 Y                    F100 300
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C       COLUMN 37-45                                  Z
C       COLUMN 46-54 INCREMENT ALONG X IN ANGSTROMS
C       COLUMN 55-63                        Y
C       COLUMN 64-67                        Z
C**** CONTINUATION CARD IF A 1 IN COLUMN 3 OF PREVIOUS CARD ****
C       COLUMN 10-18 MID-POINT IN RANGE OF X
C       COLUMN 19-27                          Y
C       COLUMN 28-36                          Z
C       COLUMN 37-45 NON-ZERO TO READ AND SUBTRACT RIGID-BODY CUMULANTS
C       COLUMN 46-54 SCALE FACTOR FOR REGULAR    CUMULANTS IN SUBTRACTION
C       COLUMN 55-63 SCALE FACTOR FOR RIGID BODY CUMULANTS IN SUBTRACTION
C       COLUMN 64-72 NON-ZERO TO READ OLD FORMAT 3K(I,J,K) CARDS
      NA1 = AIN(1)
      IF(NA1)200,200,205
  200 NA1 = 1
  205 NA2 = AIN(2)
      IF(NA2)210,210,215
  210 NA2 = NATOM
  215 DO 505 IA = NA1,NA2
C     ***** READ IN FIRST AND SECOND CUMULANT TENSORS *****
      READ(IN,2) CHEM2,SCAT,FRAC,(V6(J),J=1,3),B2(1,1),B2(2,2),B2(3,3)
     1,B2(1,2),B2(1,3),B2(2,3),ALPHA,IBE,IGM,IDL
    2 FORMAT (A6,3X,5F9.5,26X / 6F9.6,F7.4,2X,3I3)
      CONST=0.001
      IF(AIN(21))2152,2152,2151
 2151 CONST=1./41.34170
      GO TO 220
 2152 IF(IGM-1)222,217,216
  216 IF(IGM-3)220,217,220
C     ***** READ CONTRACTED GAMMA TENSOR (COVARIANT FORM) *****
  217 READ (IN,4)(C1(J),J=1,3)
    4 FORMAT (5E14.7,10X)
      IGM=3
      GO TO 222
C     ***** READ FULL GAMMA TENSOR (CONTRAVARIANT FORM) *****
  220 READ (IN,4)CIJK(1,1,1),CIJK(2,2,2),CIJK(3,3,3),CIJK(1,1,2)
     1,CIJK(1,2,2),CIJK(1,1,3),CIJK(1,3,3),CIJK(2,2,3),CIJK(2,3,3)
     2,CIJK(1,2,3)
      IGM=10
  222 IF(IDL-1)241,225,223
  223 IF(IDL-3)226,227,224
  224 IF(IDL-15)226,227,241
C     ***** READ DELTA TENSOR *****
  225 READ (IN,4) D1
      IDL=1
      GO TO 241
  226 READ (IN,4) D6(1,1),D6(2,2),D6(3,3),D6(1,2),D6(1,3),D6(2,3)
      IDL=6
      GO TO 241
  227 READ (IN,4) D15(1),D15(11),D15(15),D15(2),D15(7),D15(3),D15(10)
     1,D15(12),D15(14),D15(4),D15(6),D15(13),D15(5),D15(8),D15(9)
      IDL=15
C     ***** EXPAND BETA2 TENSOR,MULTIPLY BY 2 / (4 * PI**2) *****
  241 DO 242 I=1,3
      DO 242 J=I,3
      B2(I,J)=B2(I,J)*5.06605918E-2
  242 B2(J,I)=B2(I,J)
      IF(IGM-3)2501,243,247
  243 IF(ALPHA)500,500,244
C     ***** EXPAND CONTRACTED GAMMA TENSOR *****
  244 T1=0.2E5/ALPHA**2
      DO 245 J=1,3
  245 V2(J)=C1(J)*T1
      CALL MV(B2,V2,C1)
      DO 246 I=1,3
      DO 246 J=I,3
      DO 246 K=J,3
  246 CIJK(I,J,K)= C1(I)*B2(J,K)+C1(K)*B2(I,J)+C1(J)*B2(K,I)
  247 IF(AIN(18))235,249,235
C     ***** READ AND SUBTRACT OUT RIGID-BODY CONTRIBUTION *****
  235 READ(IN,2)CHEM3,SCAT3,FRAC,(V5(J),J=1,3),B3(1,1),B3(2,2),B3(3,3)
     1,B3(1,2),B3(1,3),B3(2,3)
      READ (IN,4)
     1GAMMA(1,1,1),GAMMA(2,2,2),GAMMA(3,3,3),GAMMA(1,1,2),GAMMA(1,2,2)
     2,GAMMA(1,1,3),GAMMA(1,3,3),GAMMA(2,2,3),GAMMA(2,3,3),GAMMA(1,2,3)
      DO 240 I = 1,3
      DO 240 J = I,3
      DO 240 K = J,3
  240 CIJK(I,J,K) = CIJK(I,J,K)*AIN(19)-GAMMA(I,J,K)*AIN(20)
  249 DO 250 I=1,3
      DO 250 J=I,3
      DO 250 K = J,3
      T1 = CIJK(I,J,K)*CONST
      CIJK(I,J,K) = T1
      CIJK(K,I,J) = T1
      CIJK(J,K,I) = T1
      CIJK(K,J,I) = T1
      CIJK(I,K,J) = T1
  250 CIJK(J,I,K) = T1
C     ***** EXPAND CONTRACTED DELTA TENSORS *****
 2501 IF(IDL-1)260,251,253
  251 D1=D1*128.0
      DO 252 I=1,3
      DO 252 J=1,3
  252 D6(I,J)=B2(I,J)*D1/3.0
  253 IF(IDL-6)256,254,260
C     ***** CONVERT TO CONTRAVARIANT FORM *****
  254 T1=28./(.01*ALPHA**3)
      DO 255 I=1,3
      DO 255 J=I,3
      D6L(I,J)=D6(I,J)*T1
  255 D6L(J,I)=D6L(I,J)
      CALL MM(B2,D6L,DA)
      CALL MM(DA,B2,D6)
C     ***** EXPAND TO 4TH ORDER TENSOR *****
  256 IJKL=0
      DO 257 I=1,3
      DO 257 J=I,3
      DO 257 K=J,3
      DO 257 L=K,3
      IJKL=IJKL+1
  257 D15(IJKL)=(B2(I,J)*D6(K,L)+B2(I,K)*D6(J,L)+B2(I,L)*D6(J,K)
     1           +B2(K,L)*D6(I,J)+B2(J,L)*D6(I,K)+B2(J,K)*D6(I,L))/7.0
C     ***** INVERT BETA MATRIX *****
  260 CALL PAXES(FLOAT(IA)*100000.+55501.,1)
C     ***** STORE IN ARRAY WITH PROPER MULTIPLICITY *****
      IJ=0
      DO 262 I=1,3
      DO 262 J=I,3
      IJ=IJ+1
      T1=2.0
      IF(I-J)262,261,262
  261 T1=1.0
  262 QQ(IJ)=Q(I,J)*T1
      IF(IDL-6)270,267,263
C     ***** CONTRACT 4TH ORDER DELTA TENSOR *****
  263 IJ=0
      DO 265 I=1,3
      DO 265 J=1,I
      IJ=IJ+1
      DQ(IJ)=0.0
      N=IJ-I
      KL=0
      DO 265 K=1,3
      N=N+I-1
      DO 265 L=1,K
      KL=KL+1
      N=N+1
  265 DQ(IJ)=DQ(IJ) + QQ(KL)*D15(N)
      IJ=0
      DO 266 I=1,3
      DO 266 J=I,3
      IJ=IJ+1
      D6(I,J)=DQ(IJ)
  266 D6(J,I)=DQ(IJ)
C     ***** CONTRACT 2NT ORDER DELTA TENSOR
  267 D1=0.0
      DO 268 I=1,3
      DO 268 J=1,3
  268 D1=D1+Q(I,J)*D6(I,J)
  270 IF(IGM-3)500,275,275
C     ***** CONTRACT GAMMA TENSOR *****
  275 DO 285 K = 1,3
      T1 = 0.0
      DO 280 J = 1,3
      VT(K,J) = PA(K,J,IA)/EV(J,IA)
      DO 280 I = 1,3
  280 T1 = T1 + CIJK(I,J,K)* Q(I,J)
  285 V1(K) = T1
      DO 290 J = 1,3
C     ***** FORM FIRST CUMULANT - MEAN DIFFERENCE VECTOR IN V5 *****
      V5(J) = V6(J) - P(J,IA) + 0.5 * ALPHA * V1(J)
      V4(J) = EV(J,IA)**2
  290 V3(J) = 1.0 / V4(J)
      WRITE(NOUT,8) (TITLE(I),I=1,18)
    8 FORMAT(1H1,10X,18A4)
      WRITE (NOUT,10)
   10 FORMAT(1H0, 9H NO. ATOM,5X,5H1L(1),6X,5H1L(2),6X,5H1L(3),  3X,33H(
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     1CONTRACTED 3K(I,I,J) =  3K(J)) =,3X,5H3K(1),6X,5H3K(2),6X,5H3K(3)/F1001950
     21H ,14X,7H3K(111),4X,7H3K(222),4X,7H3K(333),4X,7H3K(112),4X,      F1001960
     37H3K(122),4X,7H3K(113),4X,7H3K(133),4X,7H3K(223),4X,7H3K(233),3X, F1001970
     47H3K(123))                                                        F1001980
      WRITE (NOUT,12)                                                   F1001990
   12 FORMAT(1H0,22HCRYSTAL OBLIQUE SYSTEM)                             F1002000
      WRITE (NOUT,14) IA,CHEM(IA),(V5(J),J=1,3),(V1(J),J=1,3),          F1002010
     1CIJK(1,1,1),CIJK(2,2,2),CIJK(3,3,3),CIJK(1,1,2),CIJK(1,2,2),      F1002020
     2CIJK(1,1,3),CIJK(1,3,3),CIJK(2,2,3),CIJK(2,3,3),CIJK(1,2,3)       F1002030
   14 FORMAT(1H ,I3,1X,A6,3F11.8,33X,3F11.8/1H ,10X,9F11.8,F10.8)       F1002040
      WRITE (NOUT,16)                                                   F1002050
   16 FORMAT(1H0,26HREFERENCE CARTESIAN SYSTEM)                         F1002060
C     ***** TRANSFORMATION MATRIX FOR REFERENCE CARTESIAN SYSTEM *****  F1002070
      DO 295 J = 1,9                                                    F1002080
  295 PAC(J,1) = AAREV(J,1)                                             F1002090
      ISYS = 0                                                          F1002100
      GO TO 305                                                         F1002110
C     ***** REPLACE REFERENCE SYSTEM BY PRINCIPAL AXIS SYSTEM *****     F1002120
  300 CALL MM(AA,VT,PAC)                                                F1002130
      WRITE (NOUT,18)                                                   F1002140
   18 FORMAT(1H0,35HUNIT VARIANCE PRINCIPAL-AXIS SYSTEM)                F1002150
C     ***** TRANSFORM GAMMA TENSCR TO ORTHOGONAL SYSTEM *****          F1002160
  305 DO 315 N = 1,3                                                    F1002170
      DO 315 M = N,3                                                    F1002180
      DO 315 L = M,3                                                    F1002190
      T1 = 0.0                                                          F1002200
      DO 310 K = 1,3                                                    F1002210
      T2 = PAC(K,N)                                                     F1002220
      DO 310 J = 1,3                                                    F1002230
      T3 = T2 * PAC(J,M)                                                F1002240
      DO 310 I = 1,3                                                    F1002250
  310 T1 = T1 + CIJK(I,J,K)*PAC(I,L)*T3                                 F1002260
      GAMMA(L,M,N) = T1                                                 F1002270
      GAMMA(N,L,M) = T1                                                 F1002280
      GAMMA(M,N,L) = T1                                                 F1002290
      GAMMA(N,M,L) = T1                                                 F1002300
      GAMMA(L,N,M) = T1                                                 F1002310
  315 GAMMA(M,L,N) = T1                                                 F1002320
C     ***** TRANSFORM VECTORS TO ORTHOGONAL SYSTEM *****               F1002330
      DO 320 J = 1,3                                                    F1002340
      V2(J) = 0.0                                                       F1002350
      V4(J) = 0.0                                                       F1002360
      V6(J) = 0.0                                                       F1002370
      DO 320 I = 1,3                                                    F1002380
      V6(J) = V6(J) + V1(I)*PAC(I,J)                                    F1002390
  320 V4(J) = V4(J) + V5(I)*PAC(I,J)                                    F1002400
  325 WRITE (NOUT,20)IA,CHEM(IA),(V4(J),J=1,3),(V6(J),J=1,3)            F1002410
     1,GAMMA(1,1,1),GAMMA(2,2,2),GAMMA(3,3,3),GAMMA(1,1,2),GAMMA(1,2,2) F1002420
     2,GAMMA(1,1,3),GAMMA(1,3,3),GAMMA(2,2,3),GAMMA(2,3,3),GAMMA(1,2,3) F1002430
   20 FORMAT(1H ,I3,1X,A6,3F11.6,33X,3F11.6/1H ,10X,9F11.6,F10.6)       F1002440
      IF(ISYS) 330 ,330 ,340                                            F1002450
C     ***** STORE 1L(I),3K(I,J,K) AND INVERSE OF 2K(I,J) FOR EDGE SERIESF1002460
  330 CALL PAXES(FLOAT(IA)*100000.+55501.,3)                            F1002470
      IJK = 1                                                           F1002480
      DO 335  I = 1,3                                                   F1002490
      C1(I) = V4(I)                                                     F1002500
      DO 335  J = I,3                                                   F1002510
      QF(J,I) = Q(J,I)                                                  F1002520
      QF(I,J) = Q(I,J)                                                  F1002530
      DO 335  K = J,3                                                   F1002540
      C3(IJK) = GAMMA(I,J,K)*0.5                                        F1002550
  335 IJK = IJK + 1                                                     F1002560
      C3(1) = C3(1)/3.0                                                 F1002570
      C3(7) = C3(7)/3.0                                                 F1002580
      C3(10) = C3(10)/3.0                                               F1002590
      C3(5) = C3(5)*2.0                                                 F1002600
      CALL PAXES(FLOAT(IA)*100000.+55501.,-3)                           F1002610
      GO TO 350                                                         F1002620
  340 DO 345 I = 1,9                                                    F1002630
  345 Q(I,1) = AID(I,1)                                                 F1002640
C     ***** EXPAND THE CONTRACTED VECTOR *****                         F1002650
  350 IJK = 1                                                           F1002660
      DO 355 I = 1,3                                                    F1002670
      DO 355 J = I,3                                                    F1002680
      DO 355 K = J,3                                                    F1002690
      CE(IJK) = 0.2*(V6(I)*Q(J,K)+V6(J)*Q(K,I)+V6(K)*Q(I,J))            F1002700
  355 IJK = IJK + 1                                                     F1002710
      WRITE (NOUT,22) CE(1),CE(7),CE(10),CE(2),CE(4),CE(3),CE(6),CE(8)  F1002720
     1,CE(9),CE(5)                                                      F1002730
   22 FORMAT(11H XPND 3K(J),9F11.6,F10.6)                               F1002740
      ISYS = ISYS + 1                                                   F1002750
      IF(ISYS-1) 300,300,360                                            F1002760
C     ***** MULTIPLY TERMS IN BASIC UNIT OF GAMMA BY THEIR MULTIPLICITY F1002770
  360 GAMMA(1,1,2) = GAMMA(1,1,2)*3.0                                   F1002780
      GAMMA(1,2,2) = GAMMA(1,2,2)*3.0                                   F1002790
      GAMMA(1,1,3) = GAMMA(1,1,3)*3.0                                   F1002800
      GAMMA(1,3,3) = GAMMA(1,3,3)*3.0                                   F1002810
      GAMMA(2,2,3) = GAMMA(2,2,3)*3.0                                   F1002820
      GAMMA(2,3,3) = GAMMA(2,3,3)*3.0                                   F1002830
      GAMMA(1,2,3) = GAMMA(1,2,3)*6.0                                   F1002840
C     ***** CALCULATE MODE OF PROBABILITY DENSITY FUNCTION *****       F1002850
      T4 = 0.0                                                          F1002860
      DO 365 J = 1,3                                                    F1002870
      V2(J) = V4(J)-V6(J)*0.5                                           F1002880
  365 T4 = T4 + V2(J)**2                                                F1002890
      T4 = SQRT(T4)                                                     F1002900
      IF(T4-1.0) 380,380,370                                            F1002910
  370 DO 375 J = 1,3                                                    F1002920
  375 V2(J) = V2(J)/T4                                                  F1002930
  380 CALL HERMIT(V2,V4,GAMMA,PSI,CHI,EV(1,IA),1)                       F1002940
      T4 = 0.0                                                          F1002950
      DO 385 J = 1,3                                                    F1002960
      T1 = EV(J,IA)                                                     F1002970
      V2(J) = V2(J)*T1                                                  F1002980
  385 T4 = T4 + V2(J)**2                                                F1002990
      T4 = SQRT(T4)                                                     F1003000
C     ***** SHIFT POSITIONAL PARAMETERS TO MODE *****                  F1003010
      DO 395 J = 1,3                                                    F1003020
      V6(J) = P(J,IA)                                                   F1003030
      XT(J) = V6(J)                                                     F1003040
      DO 390 I = 1,3                                                    F1003050
  390 P(J,IA) = P(J,IA) + V2(I)*PA(J,I,IA)                              F1003060
  395 V3(J) = P(J,IA) - V6(J)                                           F1003070
      WRITE (NOUT,24)                                                   F1003080
   24 FORMAT(1H0,15X,6HX MEAN,5X,6HY MEAN,5X,6HZ MEAN,16X,6HX MODE,5X,  F1003090
     16HY MODE,5X,6HZ MODE,20X,12HDISPLACEMENT)                         F1003100
      WRITE (NOUT,12)                                                   F1003110
      WRITE (NOUT,26)IA,CHEM(IA),(V6(J),J=1,3),(V3(J)   ,J=1,3),T4      F1003120
   26 FORMAT(1H ,I3,1X,A6,3F11.6,11X,3F11.6,16X,F6.3,1X,9HANGSTROMS)    F1003130
      T1 = 55501. + FLOAT(IA)*100000.                                   F1003140
      CALL XYZ(T1,V2,-3)                                                F1003150
      CALL XYZ(T1,V3,3)                                                 F1003160
      DO 400 J = 1,3                                                    F1003170
  400 V3(J) = V3(J) - V2(J)                                             F1003180
      IF(AIN(3)) 415,415,405                                            F1003190
  405 DO 410 J = 1,3                                                    F1003200
  410 P(J,IA) = V6(J)                                                   F1003210
      WRITE (NOUT,28)                                                   F1003220
   28 FORMAT(1H ,   29HPOSITIONAL PARAMETERS AT MEAN)                   F1003230
      GO TO 420                                                         F1003240
  415 WRITE (NOUT,30)                                                   F1003250
   30 FORMAT(1H ,   29HPOSITIONAL PARAMETERS AT MODE)                   F1003260
C     ***** PRINT MEAN AND MODE BASED ON REFERENCE CARTESIAN SYSTEM ****F1003270
  420 WRITE (NOUT,16)                                                   F1003280
      WRITE (NOUT,26)IA,CHEM(IA),(V2(J),J=1,3),(V3(J),J=1,3),T4         F1003290
C     ***** PRINT PRINCIPAL AXES BASED ON REFERENCE CARTESIAN SYSTEM ***F1003300
      WRITE (NOUT,32)                                                   F1003310
   32 FORMAT(1H0,10X,16HRMS DISPLACEMENT, 8X,31HROW VECTORS, BASED ON REF1003320
     1FERENCE,15X,28HCOVARIANCE MATRIX (U TENSOR))                      F1003330
      CALL PAXES(T1,-3)                                                 F1003340
      WRITE (NOUT,34) (RMS(J),(PAC(I,J),I=1,3),(Q(I,J),I=1,3),J=1,3)    F1003350
   34 FORMAT(1H0,10X,F11.4,11X,3F11.6,11X,3F11.6)                       F1003360
      IF(AIN(8)) 425,505,425                                            F1003370
C     ***** CALCULATE EDGEWORTH DENSITY MAP *****                      F1003380
  425 SCAT = AMIN1(SCAT,1.0)                                            F1003390
      SCAL3=.063493636 *AIN(8)*SCAT/(EV(1,IA)*EV(2,IA)*EV(3,IA))        F1003400
      DO 430 J = 1,3                                                    F1003410
      DZ0(J) = AIN(J+11)                                                F1003420
  430 Z0(J) = AIN(J+14) - 0.5*(AIN(J+8)+1.0)*AIN(J+11)                  F1003430
      NX = AIN(9)                                                       F1003440
      NY = AIN(10)                                                      F1003450
      NZ = AIN(11)                                                      F1003460
C     ***** LOOP OVER Z OF REFERENCE SYSTEM *****                      F1003470
      DO 500 IZ = 1,NZ                                                  F1003480
      DZ1(3) = FLOAT(IZ)                                                F1003490
      Z1(3) = Z0(3) + DZ0(3)*DZ1(3)                                     F1003500
      WRITE (NOUT,36)Z1(3),CHEM(IA)                                     F1003510
   36 FORMAT (13H1 SECTION Z =,F6.3,3X,A6)                              F1003520
      DO 435 I = 1,NY                                                   F1003530
  435 HEAD(I) = Z0(2) + DZ0(2)*FLOAT(I)                                 F1003540
      WRITE (NOUT,38) (HEAD(I),I=1,NY)                                  F1003550
   38 FORMAT(9H Y(A.U.)=,22F5.2)                                        F1003560
C     ***** LOOP OVER X OF REFERENCE SYSTEM *****                      F1003570
      DO 500 IX = 1,NX                                                  F1003580
      DZ1(1) = FLOAT(IX)                                                F1003590
      Z1(1) = Z0(1) + DZ0(1)*DZ1(1)                                     F1003600
C     ***** LOOP OVER Y OF REFERENCE SYSTEM *****                      F1003610
      DO 480 IY = 1,NY                                                  F1003620
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      DZ1(2) = FLOAT(IY)                                                F1003630
      Z1(2) = Z0(2) + DZ0(2)*DZ1(2)                                     F1003640
C     ***** EVALUATE EDGEWORTH SERIES AT POINT Z1(I) *****              F1003650
      DO 440 I = 1,3                                                    F1003660
      Z2(I) = 0.0                                                       F1003670
      DO 440 J = 1,3                                                    F1003680
  440 Z2(I) = Z2(I) + Z1(J)*QF(J,I)                                     F1003690
      LILJLK = 1                                                        F1003700
      PSI = 1.0                                                         F1003710
      QUAD = 0.0                                                        F1003720
      DO 445 LI = 1,3                                                   F1003730
      Z2LI = Z2(LI)                                                     F1003740
      PSI = PSI + Z2LI*C1(LI)                                           F1003750
      QUAD = QUAD + Z2LI*Z1(LI)                                         F1003760
      DO 445 LJ = LI,3                                                  F1003770
      Z2LJ = Z2(LJ)                                                     F1003780
      ZIZJQF = Z2LI*Z2LJ - QF(LI,LJ)                                    F1003790
      DO 445 LK = LJ,3                                                  F1003800
      PSI = PSI + C3(LILJLK) * (Z2(LK)*ZIZJQF - Z2LI*QF(LK,LJ)          F1003810
     1- Z2LJ*QF(LK,LI))                                                 F1003820
  445 LILJLK = LILJLK + 1                                               F1003830
      PDF = SCAL3*EXP(-.5*QUAD)                                         F1003840
      CHI = PDF*(PSI-1.0)                                               F1003850
      PSI = PDF* PSI                                                    F1003860
C     ***** ROUND AND STORE PSI *****                                   F1003870
      T1 = PSI                                                          F1003880
      LTEMP = T1 + SIGN(0.5,T1)                                         F1003890
      IF(LTEMP)460,450,460                                              F1003900
  450 IF(T1 )455,460,460                                                F1003910
  455 LTEMP = -0                                                        F1003920
  460 LINE(IY,1) = LTEMP                                                F1003930
C     ***** ROUND AND STORE CHI *****                                   F1003940
      T1 = CHI                                                          F1003950
      LTEMP = T1 + SIGN(0.5,T1)                                         F1003960
      IF(LTEMP)475,465,475                                              F1003970
  465 IF(T1 )470,475,475                                                F1003980
  470 LTEMP = -0                                                        F1003990
  475 LINE(IY,2) = LTEMP                                                F1004000
  480 CONTINUE                                                          F1004010
C     ***** PRINT PSI AND CHI IF AIN(4).EQ.0 , ONLY PSI IF +, CHI IF - *F1004020
      IF(AIN(4)) 495,485,490                                            F1004030
  485 WRITE (NOUT,40)                                                   F1004040
      WRITE (NOUT,44)Z1(1),(LINE(J,1),J=1,NY)                           F1004050
      WRITE (NOUT,46)Z1(1),(LINE(J,2),J=1,NY)                           F1004060
      GO TO 500                                                         F1004070
  490 WRITE (NOUT,42)                                                   F1004080
      WRITE (NOUT,44)Z1(1),(LINE(J,1),J=1,NY)                           F1004090
      GO TO 500                                                         F1004100
  495 WRITE (NOUT,42)                                                   F1004110
      WRITE (NOUT,46)Z1(1),(LINE(J,2),J=1,NY)                           F1004120
   40 FORMAT(1H )                                                       F1004130
   42 FORMAT(1H0)                                                       F1004140
   44 FORMAT(3H XP, F6.3,22I5)                                          F1004150
   46 FORMAT(3H XC, F6.3,22I5)                                          F1004160
  500 CONTINUE                                                          F1004170
  505 CONTINUE                                                          F1004180
      RETURN                                                            F1004190
      END                                                               F1004200


      SUBROUTINE HERMIT(X,U,GAMMA,PSI,CHI,RMS,ITYPE)
C     ***** SUBROUTINE TO REFINE MODE *****                             HERM  10
      DIMENSION A(3,3),X(3),Y(3),GAMMA(3,3,3),H(6,3)        ,KH(4),V1(3) HERM  20
      DIMENSION  JT(5,10),IT(5),VALU(3),VECT(3,3),RMS(3),U(3)           HERM  30
C     ***** ITYPE=0, PSI, CHI CALC/.GT.0 MAXIMUM PHI/.LT.0 MAXIMUM CHI  HERM  40
      ICYCLE = 0                                                        HERM  50
      IF(ITYPE)205,200,210                                              HERM  60
  200 ASSIGN 435 TO NBY1                                                HERM  70
      ASSIGN 300 TO NBY2                                                HERM  80
      ASSIGN 435 TO NBY3                                                HERM  90
      ILAST = 1                                                         HERM 100
      GO TO 220                                                         HERM 110
  205 ASSIGN 435 TO NBY3                                                HERM 120
      ASSIGN 290 TO NBY2                                                HERM 130
      GO TO 215                                                         HERM 140
  210 ASSIGN 330 TO NBY3                                                HERM 150
      ASSIGN 285 TO NBY2                                                HERM 160
  215 ASSIGN 260 TO NBY1                                                HERM 170
      ILAST = 4                                                         HERM 180
  220 ICYCLE = ICYCLE + 1                                               HERM 190
      ASSIGN 235 TO I5BY                                                HERM 200
      ASSIGN 245 TO I4BY                                                HERM 210
      ASSIGN 270 TO I3BY                                                HERM 220
      ASSIGN 315 TO I2BY                                                HERM 230
      ASSIGN 355 TO I1BY                                                HERM 240
      PSI = 1.0                                                         HERM 250
C     ***** GENERATE H0,H1,...,H5 FOR X(IX),IX=1,3 *****                HERM 260
      DO 230 IX = 1,3                                                   HERM 270
      H(1,IX) = 1.0                                                     HERM 280
      XH = X(IX)                                                        HERM 290
      H(2,IX) = XH                                                      HERM 300
      HI = 1.0                                                          HERM 310
      DO 225 IH = 2,5                                                   HERM 320
      H(IH+1,IX) = XH*H(IH,IX) - HI*H(IH-1,IX)                          HERM 330
  225 HI = HI + 1.0                                                     HERM 340
      Y(IX) = 0.0                                                       HERM 350
      KH(IX) = 1                                                        HERM 360
      DO 230 J = 1,3                                                    HERM 370
C     ***** REDEFINE HERMITE POLYNOMIALS WITHOUT (-1)**N FACTOR *****   HERM 380
      JX2 = J*2                                                         HERM 390
      H(JX2,IX) = -H(JX2,IX)                                            HERM 400
  230 A(J,IX) = 0.0                                                     HERM 410
      KH(4) = 1                                                         HERM 420
C     ***** FORM TENSORS OF HERMITE POLYNOMIALS *****                   HERM 430
      DO 455 I1 = 1,ILAST                                               HERM 440
      I1M1 = I1 - 1                                                     HERM 450
      IT(1) = I1M1                                                      HERM 460
      KH(I1) = KH(I1) + 1                                               HERM 470
      DO 450 I2 =I1,ILAST                                               HERM 480
      I2M1 = I2 - 1                                                     HERM 490
      IT(2) = I2M1                                                      HERM 500
      KH(I2) = KH(I2) + 1                                               HERM 510
      DO 445 I3 = I2,4                                                  HERM 520
      I3M1 = I3 - 1                                                     HERM 530
      IT(3) = I3M1                                                      HERM 540
      KH(I3) = KH(I3) + 1                                               HERM 550
      DO 440 I4 = I3,4                                                  HERM 560
      I4M1 = I4 - 1                                                     HERM 570
      IT(4) = I4M1                                                      HERM 580
      KH(I4) = KH(I4) + 1                                               HERM 590
      DO 435 I5 = I4,4                                                  HERM 600
      I5M1 = I5-1                                                       HERM 610
      IT(5) = I5M1                                                      HERM 620
      KH(I5) = KH(I5) + 1                                               HERM 630
C     *****SKIP ZERO ORDER TERM *****                                   HERM 640
      GO TO I5BY,(235,240)                                              HERM 650
  235 ASSIGN 240 TO I5BY                                                HERM 660
      GO TO 435                                                         HERM 670
  240 K1 = KH(2)                                                        HERM 680
      K2 = KH(3)                                                        HERM 690
      K3 = KH(4)                                                        HERM 700
      TERM = H(K1,1)*H(K2,2)*H(K3,3)                                    HERM 710
      GO TO I4BY,(245,265)                                              HERM 720
  245 IF(I4M1) 255,255,250                                              HERM 730
  250 ASSIGN 265 TO I4BY                                                HERM 740
      GO TO 265                                                         HERM 750
C     ***** USE H(I) *****                                              HERM 760
C     ***** SUM SECOND PART OF PSI *****                                HERM 770
  255 PSI = PSI - TERM * U(I5M1)                                        HERM 780
      GO TO NBY1,(260,435)                                              HERM 790
C     ***** SUM FIRST PART OF VECTOR OF FIRST DERIVITIVES *****         HERM 800
  260 Y(I5M1) = Y(I5M1) - TERM                                          HERM 810
      GO TO 435                                                         HERM 820
  265 GO TO I3BY,(270,305)                                              HERM 830
  270 IF(I3M1) 280,280,275                                              HERM 840
  275 ASSIGN 305 TO I3BY                                                HERM 850
      GO TO 305                                                         HERM 860
C     ***** USE H(I)H(J) *****                                          HERM 870
  280 GO TO NBY2,(285,290,300)                                          HERM 880
C     ***** SUM FIRST PART OF MATRIX OF SECOND DERIVITIVES *****        HERM 890
  285 A(I4M1,I5M1) = A(I4M1,I5M1) + TERM                                HERM 900
C     ***** SUM SECOND PART OF VECTOR OF FIRST DERIVITIVES *****        HERM 910
  290 Y(I5M1) = Y(I5M1) + TERM * U(I4M1)                                HERM 920
      IF(I5M1-I4M1)435,435,295                                          HERM 930
  295 Y(I4M1) = Y(I4M1) + TERM * U(I5M1)                                HERM 940
      GO TO 435                                                         HERM 950
C     ***** SKIP H(I)H(J) PART IF CALCULATING PHI ONLY *****            HERM 960
  300 KH(I5) = KH(I5) - 1                                               HERM 970
      KH(I4) = KH(I4) - 1                                               HERM 980
      GO TO 445                                                         HERM 990
C     ***** CALCULATE CONSTANT*GAMMA(I,J,K)*HERMITE(I,J,K) *****        HERM1000
  305 TERM2 = GAMMA(I3M1,I4M1,I5M1)*TERM*0.16666667                     HERM1010
  310 GO TO I2BY,(315,350)                                              HERM1020
  315 IF(I2M1) 325,325,320                                              HERM1030
  320 ASSIGN 350 TO I2BY                                                HERM1040
      GO TO 350                                                         HERM1050
                                                                        HERM1060
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C     ***** USE H(I)H(J)H(K)  *****                                      HERM1070
C     ***** SUM THIRD PART OF PSI *****                                  HERM1080
  325 PSI = PSI - TERM2                                                   HERM1090
      GO TO NBY3,(330,435)                                                HERM1100
C     ***** SUM SECOND PART OF MATRIX OF SECOND DERIVITIVES *****        HERM1110
  330 A(I4M1,I5M1) = A(I4M1,I5M1) - TERM * U(I3M1)                        HERM1120
      IF(I5M1-I4M1)340,340,335                                            HERM1130
  335 A(I3M1,I4M1) = A(I3M1,I4M1) - TERM * U(I5M1)                        HERM1140
  340 IF(I4M1-I3M1)435,435,345                                            HERM1150
  345 A(I3M1,I5M1) = A(I3M1,I5M1) - TERM * U(I4M1)                        HERM1160
      GO TO 435                                                           HERM1170
  350 GO TO I1BY,(355,395)                                                HERM1180
  355 IF(I1M1) 365,365,360                                                HERM1190
  360 ASSIGN 395 TO I1BY                                                  HERM1200
      GO TO 395                                                           HERM1210
C     ***** USE H(I)H(J)H(K)H(L)  *****                                  HERM1220
C     ***** SUM THIRD PART OF VECTOR OF FIRST DERIVITIVES *****          HERM1230
  365 Y(I2M1) = Y(I2M1) + TERM2                                           HERM1240
      IF(I5M1-I4M1)375,375,370                                            HERM1250
  370 Y(I5M1) = Y(I5M1) + GAMMA(I2M1,I3M1,I4M1)*TERM*0.16666667           HERM1260
  375 IF(I4M1-I3M1)385,385,380                                            HERM1270
  380 Y(I4M1) = Y(I4M1) + GAMMA(I2M1,I3M1,I5M1)*TERM*0.16666667           HERM1280
  385 IF(I3M1-I2M1)435,435,390                                            HERM1290
  390 Y(I3M1) = Y(I3M1) + GAMMA(I2M1,I4M1,I5M1)*TERM*0.16666667           HERM1300
      GO TO 435                                                           HERM1310
C     ***** USE H(I)H(J)H(K)H(L)H(M)  *****                              HERM1320
C     ***** SUM THIRD PART OF MATRIX OF SECOND DERIVITIVES *****         HERM1330
C     ***** SET UP ORDERED PERMUTATIONS OF I1,I2,I3,I4,I5 BY 2 S, 3 S **HERM1340
  395 LT = 0                                                              HERM1350
      LB = 11                                                             HERM1360
      DO 410 I=1,4                                                        HERM1370
      IP1 = I+1                                                           HERM1380
      DO 410 J=IP1,5                                                      HERM1390
      LT = LT+1                                                           HERM1400
      JT(1,LT) = IT(I)                                                    HERM1410
      JT(2,LT) = IT(J)                                                    HERM1420
      IF(J-4)400,400,410                                                  HERM1430
  400 JP1 = J+1                                                           HERM1440
      DO 405 K=JP1,5                                                      HERM1450
      LB = LB-1                                                           HERM1460
      JT(3,LB) = IT(I)                                                    HERM1470
      JT(4,LB) = IT(J)                                                    HERM1480
  405 JT(5,LB) = IT(K)                                                    HERM1490
  410 CONTINUE                                                            HERM1500
C     ***** FIND UNIQUE ORDERED PERMUTATIONS OF I1,I2,I3,I4,I5 BY 2,3 S HERM1510
      J1 = 0                                                              HERM1520
      J2 = 0                                                              HERM1530
      J5 = 0                                                              HERM1540
      DO 430 J=1,10                                                       HERM1550
      IF((J1-3)*(J5-1))415,435,415                                        HERM1560
  415 IF(J1-JT(1,J))425,420,425                                           HERM1570
  420 IF(J2-JT(2,J))425,430,425                                           HERM1580
  425 J1 = JT(1,J)                                                        HERM1590
      J2 = JT(2,J)                                                        HERM1600
      J3 = JT(3,J)                                                        HERM1610
      J4 = JT(4,J)                                                        HERM1620
      J5 = JT(5,J)                                                        HERM1630
      A(J1,J2) = A(J1,J2) - GAMMA(J3,J4,J5)*TERM*0.16666667               HERM1640
  430 CONTINUE                                                            HERM1650
  435 KH(I5) = KH(I5) - 1                                                 HERM1660
  440 KH(I4) = KH(I4) - 1                                                 HERM1670
  445 KH(I3) = KH(I3) - 1                                                 HERM1680
  450 KH(I2) = KH(I2) - 1                                                 HERM1690
  455 KH(I1) = KH(I1) - 1                                                 HERM1700
C     ***** FILL OUT MATRIX A AND MULTIPLY A,Y AND PSI BY NORMAL DENSITYHERM1710
      DEN = 0.063493636 * EXP(-.5*(X(1)**2+X(2)**2+X(3)**2))              HERM1720
      PSI = PSI * DEN                                                     HERM1730
      CHI = PSI - DEN                                                     HERM1740
      IF(ITYPE)460,500,460                                                HERM1750
C     ***** NEGATE DENSITY FOR POSITIVE MATRIX A ON MAXIMA SEARCH ***** HERM1760
  460 DEN = -DEN                                                          HERM1770
      DO 470 I = 1,3                                                      HERM1780
      DO 465 J = I,3                                                      HERM1790
      A(I,J) = A(I,J)*DEN                                                 HERM1800
  465 A(J,I) = A(I,J)                                                     HERM1810
  470 Y(I) = Y(I) * DEN                                                   HERM1820
C     ***** CHECK EIGENVALUES OF MATRIX A *****                          HERM1830
      CALL EIGEN(A,VALU,VECT)                                             HERM1840
      IF(VALU(1))495,495,475                                              HERM1850
C     *****CALCULATE SHIFT VECTOR *****                                   HERM1860
  475 CALL AXEQB(A,V1,Y,1)                                                HERM1870
C     ***** CALCULATE LENGTH OF SHIFT VECTOR *****                        HERM1880
      T1 = 0.0                                                            HERM1890
      DO 480 J = 1,3                                                      HERM1900
      T1 = T1 + (V1(J)*RMS(J))**2                                         HERM1910
  480 X(J) = X(J) + V1(J)                                                 HERM1920
      IF(T1-1.0E-10)500,485,485                                           HERM1930
C     ***** ERROR IF SHIFT IS .GE. 0.3 A *****                           HERM1940
  485 IF(T1-0.09)490,495,495                                              HERM1950
  490 IF(ICYCLE-20)220,495,495                                            HERM1960
  495 PRINT 2,ICYCLE,VALU                                                 HERM1970
    2 FORMAT(22H0MODE FAILURE ON CYCLE,I3,3E20.5)                         HERM1980
      PRINT 4,PSI,CHI,T1,V1,X,VALU,Y,A,H                                  HERM1990
    4 FORMAT(1H0/(1H ,6E19.8))                                            HERM2000
  500 RETURN                                                              HERM2010
      END                                                                 HERM2020


      SUBROUTINE LAP500(NTYPE)                                            LAP5  10
C     ***** STORE PROJECTED ATOM CONICS AND BOND QUADRANGLES *****       LAP5  20
      DIMENSION QC(3,3),QD(3,3),VD1(3),VD2(3)                             LAP5  30
C     ***** DOUBLE PRECISION FOR VERY SMALL ATOMS AND SHORT WORDLENGTH *LAP5  40
C     ***** IN GENERAL, DOUBLE PRECISION IS NOT REQUIRED *****           LAP5  50
      REAL*8 QC,QD,VD1,VD2,TD1,TD2,TD3                                    LAP5  60
C     ***** JUST REMOVE THE PRECEEDING REAL*8 CARD TO MAKE SINGLE PREC   LAP5  70
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER,  LAP5  80
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)          LAP5  90
      REAL*8 CHEM                                                         LAP5 100
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      LAP5 110
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) LAP5 120
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)  LAP5 130
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  LAP5 140
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)    LAP5 150
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    LAP5 160
      DIMENSION XLNG(3),XO(3),XT(3)                                       LAP5 170
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D    LAP5 180
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD  LAP5 190
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALILAP5 200
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    LAP5 210
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                  LAP5 220
C     ***** ELIMINATE ALL PREVIOUSLY STORED LOCAL OVERLAP INFORMATION **LAP5 230
      NCOVER=0                                                            LAP5 240
      NQOVER=0                                                            LAP5 250
      IF(NTYPE)420,195,195                                                LAP5 260
C     ***** ELIMINATE ALL PREVIOUSLY STORED GLOBAL OVERLAP INFORMATION *LAP5 270
  195 NCONIC=0                                                            LAP5 280
      NQUAD=0                                                             LAP5 290
      IF(NTYPE)420,420,200                                                LAP5 300
C     ***** CONSTANT FOR OVERLAP MARGIN (WHITE MARGIN AT OVERLAP) ***** LAP5 310
  200 IF(AIN(1))205,215,210                                               LAP5 320
C     ***** NEGATIVE NUMBER OR POSITIVE INTEGER GIVES OVMRGN=0.0 *****  LAP5 330
  205 OVMRGN=0.0                                                          LAP5 340
      GO TO 220                                                           LAP5 350
C     ***** SET OVERLAP MARGIN WIDTH DIRECTLY IN INCHES *****            LAP5 360
  210 OVMRGN=AIN(1)-AINT(AIN(1))                                          LAP5 370
      GO TO 220                                                           LAP5 380
C      ***** DEFAULT OPTION, OVERLAP MARGIN WIDTH AS A FUNCTION OF SCALILAP5 390
  215 OVMRGN=AMAX1(SQRT(SCAL1)*0.030,0.025)                               LAP5 400
  220 WRITE (NOUT,2) OVMRGN                                               LAP5 410
    2 FORMAT(1H0,10X,17HOVERLAP MARGIN IS, F6.3,5H INCH)                  LAP5 420
  225 IF(LATM) 230,230,235                                                LAP5 430
  230 NG=12                                                               LAP5 440
      CALL ERPNT(0.,510+NJ2)                                              LAP5 450
      GO TO 420                                                           LAP5 460
C     ***** SORT ATOMS LIST BY -VIEWDISTANCE OR BY Z PARAMETER           LAP5 470
  235 IF(VIEW) 250,250,240                                                LAP5 480
C     ***** CALCULATE VIEWDISTANCES**2 *(-1) IF VIEW.GT.ZERO *****      LAP5 490
  240 DO 245 I=1,LATM                                                     LAP5 500
      CALL XYZ(ATOMS(1,I),V3,2)                                           LAP5 510
      V3(3)=V3(3)-VIEW                                                    LAP5 520
  245 ATOMS(4,I)=-VV(V3,V3)                                               LAP5 530
      GO TO 260                                                           LAP5 540
C     ***** STORE CARTESIAN COORDINATES IF VIEW.EQ.ZERO *****            LAP5 550
  250 DO 255 I=1,LATM                                                     LAP5 560
  255 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                   LAP5 570
C     ***** SORTING PROCEDURE BY SHELL, COMM ACM 2,30 (1959) *****       LAP5 580
  260 M=LATM                                                              LAP5 590
  265 M=M/2                                                               LAP5 600
      IF(M)300,300,270                                                    LAP5 610
  270 K=LATM-M                                                            LAP5 620
      J=1                                                                 LAP5 630
  275 I=J                                                                 LAP5 640
  280 IM=I+M                                                              LAP5 650
      IF(ATOMS(4,I)-ATOMS(4,IM))295,295,285                               LAP5 660
  285 DO 290 L=1,4,3                                                      LAP5 670
      T1=ATOMS(L,I)                                                       LAP5 680
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      ATOMS(L,I)=ATOMS(L,IM)                                            LAP5 690
  290 ATOMS(L,IM)=T1                                                    LAP5 700
      I=I-M                                                             LAP5 710
      IF(I)295,295,280                                                  LAP5 720
  295 J=J+1                                                             LAP5 730
      IF(J-K)275,275,265                                                LAP5 740
C     ***** LOOP THROUGH ALL ATOMS IN SORTED ATOMS LIST *****           LAP5 750
  300 DO 405 IA=1,LATM                                                  LAP5 760
      CALL XYZ(ATOMS(1,IA),ATOMS(2,IA),2)                               LAP5 770
      CALL PAXES(ATOMS(1,IA),2)                                         LAP5 780
      DO 305 J=1,3                                                      LAP5 790
      V1(J)=ATOMS(J+1,IA)                                               LAP5 800
      VD1(J)=V1(J)                                                      LAP5 810
      DO 305 K=1,3                                                      LAP5 820
  305 QD(J,K)=Q(J,K)                                                    LAP5 830
      IF(VIEW)340,340,310                                               LAP5 840
C     ***** CALCULATE ENVELOPING CONE WITH ORIGIN AT VIEWPOINT *****   LAP5 850
  310 V1(3)=V1(3)-VIEW                                                  LAP5 860
      VD1(3)=V1(3)                                                      LAP5 870
C     ***** FORM COFACTOR MATRIX *****                                 LAP5 880
      DO 315 J=1,3                                                      LAP5 890
      J1=MOD(J,3)+1                                                     LAP5 900
      J2=MOD(J+1,3)+1                                                   LAP5 910
      DO 315 K=J,3                                                      LAP5 920
      K1=MOD(K,3)+1                                                     LAP5 930
      K2=MOD(K+1,3)+1                                                   LAP5 940
      QC(J,K)= QD(J1,K1)*QD(J2,K2)-QD(J1,K2)*QD(J2,K1)                  LAP5 950
  315 QC(K,J)=QC(J,K)                                                   LAP5 960
C     ***** FORM POLARIZED COFACTOR MATRIX AND ADD TO ELLIPSOID MATRIX *LAP5 970
      TD2=-SCL**2                                                       LAP5 980
C     ***** TD1 IS AN ARBITRARY SCALING FACTOR *****                   LAP5 990
      TD1=VMV(V1,Q,V1)                                                  LAP51000
      DO 325 J=1,3                                                      LAP51010
      J1=MOD(J,3)+1                                                     LAP51020
      J2=MOD(J+1,3)+1                                                   LAP51030
      DO 320 K=J,3                                                      LAP51040
      K1=MOD(K,3)+1                                                     LAP51050
      K2=MOD(K+1,3)+1                                                   LAP51060
      QD(J,K)=((VD1(J2)*(QC(J1,K1)*VD1(K2)-QC(J1,K2)*VD1(K1))           LAP51070
     1 +VD1(J1)*(VD1(K1)*QC(J2,K2)-VD1(K2)*QC(J2,K1)))+TD2*QD(J,K))/TD1 LAP51080
  320 QD(K,J)=QD(J,K)                                                   LAP51090
C     ***** PROJECTED ELLIPSE IN HOMOGENEOUS COORD OF WORKING SYSTEM ***LAP51100
      QD(J,3)=-QD(J,3)*VIEW                                             LAP51110
  325 QD(3,J)=-QD(3,J)*VIEW                                             LAP51120
C     ***** PROJECT CENTER OF ATOM ONTO PROJECTION PLANE *****         LAP51130
      TD1=-VIEW/VD1(3)                                                  LAP51140
      VD2(1)=VD1(1)*TD1                                                 LAP51150
      VD2(2)=VD1(2)*TD1                                                 LAP51160
C     ***** TRANSFORM TO NEW ORIGIN TO IMPROVE CONDITION OF MATRIX Q ***LAP51170
      DO 330 J=1,3                                                      LAP51180
      DO 330 K=1,2                                                      LAP51190
  330 QD(J,3)=QD(J,3)+QD(J,K)*VD2(K)                                    LAP51200
      DO 335 J=1,3                                                      LAP51210
      DO 335 K=1,2                                                      LAP51220
  335 QD(3,J)=QD(3,J)+VD2(K)*QD(K,J)                                    LAP51230
      V6(1)=XO(1)+VD2(1)                                                LAP51240
      V6(2)=XO(2)+VD2(2)                                                LAP51250
      GO TO 355                                                         LAP51260
C     ***** CALCULATE ENVELOPING CYLINDER ALONG Z OF WORKING SYSTEM ****LAP51270
  340 DO 345 J=1,2                                                      LAP51280
      DO 345 K=1,2                                                      LAP51290
  345 QD(J,K)=QD(J,K)-QD(J,3)*QD(K,3)/QD(3,3)                           LAP51300
      DO 350 J=1,2                                                      LAP51310
      QD(J,3)=0.0                                                       LAP51320
      QD(3,J)=0.0                                                       LAP51330
  350 V6(J)=XO(J)+ATOMS(J+1,IA)                                         LAP51340
C     ***** PROJECTED ELLIPSE IN HOMOGENEOUS COORD ABOUT CENTER OF ATOM LAP51350
      QD(3,3)=-SCL**2                                                   LAP51360
C     ***** FIT RECTANGLE AROUND ELLIPSE ALLOWING OVERLAP MARGIN *****  LAP51370
C     ***** FORM MATRIX OF COFACTORS *****                             LAP51380
  355 DO 360 J=1,3                                                      LAP51390
      J1=MOD(J,3)+1                                                     LAP51400
      J2=MOD(J+1,3)+1                                                   LAP51410
      DO 360 K=J,3                                                      LAP51420
      K1=MOD(K,3)+1                                                     LAP51430
      K2=MOD(K+1,3)+1                                                   LAP51440
  360 QC(J,K)= QD(J1,K1)*QD(J2,K2)-QD(J1,K2)*QD(J2,K1)                  LAP51450
C     ***** RESCALE MATRIX OF COFACTORS SO THAT QC(3,3)=1.0 *****      LAP51460
      DO 365 J=1,3                                                      LAP51470
      DO 365 K=J,3                                                      LAP51480
      QC(J,K)= QC(J,K)/QC(3,3)                                          LAP51490
  365 QC(K,J)=QC(J,K)                                                   LAP51500
      TD2=QD(3,3)                                                       LAP51510
      NDG=0                                                             LAP51520
      DO 385 J=1,2                                                      LAP51530
C     ***** SOLVE QUADRATIC EQUATION *****                             LAP51540
      T1 =QC(3,J)**2-QC(J,J)                                            LAP51550
      IF(T1)370,370,375                                                 LAP51560
C     ***** ROUNDOFF PROBLEMS, RESET LIMITS IN X OR Y *****            LAP51570
  370 NDG=1                                                             LAP51580
      V5(J)=0.001+OVMRGN                                                LAP51590
      GO TO 380                                                         LAP51600
  375 V5(J)=  SQRT(T1)+OVMRGN                                           LAP51610
      V6(J)=V6(J)+QC(3,J)                                               LAP51620
      TD2=TD2+QD(3,J)*QC(3,J)                                           LAP51630
  380 CONIC(2*J-1,IA)=V6(J)-V5(J)                                       LAP51640
  385 CONIC(2*J,IA)=V6(J)+V5(J)                                         LAP51650
      IF(NDG)390,390,395                                                LAP51660
  390 IF(TD2)400,395,395                                                LAP51670
C     ***** ELLIPSE IMAGINARY DUE TO ROUNDOFF, RESET TO REAL VALUE *****LAP51680
  395 CONIC(5,IA)=1.0/((CONIC(2,IA)-CONIC(1,IA))*0.5)**2                LAP51690
      CONIC(6,IA)=0.0                                                   LAP51700
      CONIC(7,IA)=1.0/((CONIC(4,IA)-CONIC(3,IA))*0.5)**2                LAP51710
      GO TO 405                                                         LAP51720
C     ***** STORE NORMALIZED QUADRATIC COEFFICIENTS FOR ELLIPSE *****  LAP51730
C     ***** SCALED BY OVERLAP MARGIN PARAMETER *****                   LAP51740
  400 TD3= -(1.0-2.0*OVMRGN/(V5(1)+V5(2)))**2 /TD2                      LAP51750
      CONIC(5,IA)=QD(1,1)*TD3                                           LAP51760
      CONIC(6,IA)=QD(1,2)*TD3                                           LAP51770
      CONIC(7,IA)=QD(2,2)*TD3                                           LAP51780
  405 CONTINUE                                                          LAP51790
      NCONIC=LATM                                                       LAP51800
C     ***** PRINT OUT SORTED ATOMS ARRAY *****                         LAP51810
      WRITE (NOUT,4)(ATOMS(1,J),J=1,LATM)                               LAP51820
    4 FORMAT(1H0,10X,30HCONTENTS OF SORTED ATOMS ARRAY/(15X,10F10.0))   LAP51830
C     ***** STORE BOND QUADRANGLES IF SEARCH CODES ARE GIVEN *****     LAP51840
      IF(NCD)420,420,410                                                LAP51850
C     ***** GENERATE PSEUDO-INSTRUCTION 822 TO CALCULATE BONDS *****   LAP51860
  410 NJ2=22                                                            LAP51870
      CALL P800                                                         LAP51880
      IF(NQUAD)420,420,415                                              LAP51890
C     ***** PRINT OUT NUMBER OF BOND QUADRANGLES STORED *****          LAP51900
C     ***** PRINT OUT QUADRANGLE IDENTIFICATION ARRAY *****            LAP51910
  415 WRITE (NOUT,6)NQUAD,(QUAD(9,J),J=1,NQUAD)                         LAP51920
    6 FORMAT(1H0,10X,27HBOND OVERLAP ARRAY CONTAINS,I4,23H BONDS (MAXIMULAP51930
     1M IS 599)/  11X,  66HATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE LAP51940
     2IN SORTED ATOMS ARRAY/(15X,10F10.0))                              LAP51950
  420 RETURN                                                            LAP51960
      END                                                               LAP51970


      SUBROUTINE LAP700(NA,ICQ)                                         LAP7  10
      DIMENSION DETER(2),QA(3,3,2),QC(3,3,2),V12(3,2),YMIN(2),YMAX(2)   LAP7  20
      DIMENSION OVMR(2)                                                 LAP7  30
C     ***** IN GENERAL, DOUBLE PRECISION IS NOT REQUIRED *****         LAP7  40
C     ***** BUT IN CASE OF TROUBLE, ACTIVATE THE CD COMMENT CARDS ***** LAP7  50
      REAL*8 AOV3,AOV3SQ,BOV3,DETER,PI,PHI,POV3,POV3CU,QA,QC,QOV2,QOV2SQLAP7  60
      REAL*8 ROOT,TD                                                    LAP7  70
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER, LAP7  80
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)         LAP7  90
      REAL*8 CHEM                                                       LAP7 100
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    LAP7 110
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)LAP7 120
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) LAP7 130
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAP7 140
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   LAP7 150
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   LAP7 160
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAP7 170
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   LAP7 180
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD LAP7 190
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAP7 200
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAP7 210
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                LAP7 220
      PI=3.1415926535897932                                             LAP7 230
CS    PI=3.141593                                                       LAP7 240
      ICQ=0                                                             LAP7 250
      NCOVER=0                                                          LAP7 260
      NQOVER=0                                                          LAP7 270
      OVMR(1)=OVMRGN                                                    LAP7 280
      OVMR(2)=0.0                                                       LAP7 290
      IF(NCONIC-NA)200,200,205                                          LAP7 300
  200 RETURN                                                            LAP7 310
C     ***** ROUGH CHECK FOR OVERLAPPING ATOMS *****                    LAP7 320
  205 DO  210 J=1,2                                                     LAP7 330
      YMIN(J)=CONIC(2*J-1,NA)                                           LAP7 340
  210 YMAX(J)=CONIC(2*J,NA)                                             LAP7 350
      L=0                                                               LAP7 360
      DO 420 IA=NA,NCONIC                                               LAP7 370
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      IF(IA-NA)230,230,215                                              LAP7 380
  215 DO 225 J=1,2                                                      LAP7 390
      IF(YMAX(J)-CONIC(2*J-1,IA))420,420,220                            LAP7 400
  220 IF(YMIN(J)-CONIC(2*J,IA))225,420,420                              LAP7 410
  225 CONTINUE                                                          LAP7 420
C     ***** EXACT CHECK FOR OVERLAPPING ATOMS *****                     LAP7 430
  230 IF(L-1)235,235,240                                                LAP7 440
  235 L=L+1                                                             LAP7 450
  240 CALL LAPCON(CONIC(1,IA),DA,V12(1,L),OVMR(L))                      LAP7 460
      DO 245 J=1,3                                                      LAP7 470
      DO 245 K=1,3                                                      LAP7 480
  245 QA(J,K,L)=DA(J,K)                                                 LAP7 490
C     ***** CALCULATE COFACTORS AND DETERMINANTS *****                  LAP7 500
      DETER(L)=0.0                                                      LAP7 510
      DO 250 J=1,3                                                      LAP7 520
      J1=MOD(J+3,3)+1                                                   LAP7 530
      J2=MOD(J+1,3)+1                                                   LAP7 540
      DO 250 K=1,3                                                      LAP7 550
      K1=MOD(K+3,3)+1                                                   LAP7 560
      K2=MOD(K+1,3)+1                                                   LAP7 570
      TD=QA(J1,K1,L)*QA(J2,K2,L)-QA(J1,K2,L)*QA(J2,K1,L)                LAP7 580
      DETER(L)=DETER(L)+TD*QA(J,K,L)                                    LAP7 590
  250 QC(J,K,L)=TD                                                      LAP7 600
C     ***** DETER(L) IS THE DETERMINANT TIMES 3 *****                   LAP7 610
      IF(L-1)420,420,255                                                LAP7 620
C     ***** FORM CHARACTERISTIC EQUATION AND EXAMINE ITS ROOTS *****    LAP7 630
  255 AOV3=0.0                                                          LAP7 640
      BOV3=0.0                                                          LAP7 650
      DO 260 J=1,3                                                      LAP7 660
      DO 260 K=1,3                                                      LAP7 670
      AOV3=AOV3+QC(J,K,2)*QA(J,K,1)                                     LAP7 680
  260 BOV3=BOV3+QC(J,K,1)*QA(J,K,2)                                     LAP7 690
      AOV3=AOV3/ DETER(2)                                               LAP7 700
      AOV3SQ=AOV3**2                                                    LAP7 710
      BOV3=BOV3/ DETER(2)                                               LAP7 720
      POV3=BOV3-AOV3SQ                                                  LAP7 730
      QOV2=AOV3*(AOV3SQ-BOV3*1.5D0)+DETER(1)/(DETER(2)*2.0D0)           LAP7 740
CS    QOV2=AOV3*(AOV3SQ-BOV3*1.5  )+DETER(1)/(DETER(2)*2.0  )           LAP7 750
C     ***** CHECK DISCRIMINANT OF CHARACTERISTIC CUBIC EQUATION *****   LAP7 760
      ITYPE=0                                                           LAP7 770
      POV3CU=POV3**3                                                    LAP7 780
      QOV2SQ=QOV2**2                                                    LAP7 790
      IF(POV3CU+QOV2SQ)270,310,265                                      LAP7 800
  265 IF(POV3CU*1.00001 +QOV2SQ)310,310,400                             LAP7 810
  270 IF(POV3CU+1.00001 *QOV2SQ)275,310,310                             LAP7 820
C     ***** THREE REAL ROOTS, ALL DIFFERENT *****                       LAP7 830
  275 ITYPE=1                                                           LAP7 840
C     ***** NO INTERSECTION IF A/3 AND B/3 INVARIANTS ARE NEGATIVE *****LAP7 850
      IF(AOV3)280,285,285                                               LAP7 860
  280 IF(BOV3)420,285,285                                               LAP7 870
C     ***** CALCULATE ONE ROOT OF CHARACTERISTIC CUBIC EQUATION *****   LAP7 880
  285 IF(QOV2)295,290,295                                               LAP7 890
  290 PHI=PI/2.0D0                                                      LAP7 900
CS290 PHI=PI/2.0                                                        LAP7 910
      GO TO 305                                                         LAP7 920
  295 PHI=DATAN(-DSQRT(-POV3CU-QOV2SQ)/QOV2)                            LAP7 930
CS295 PHI= ATAN(- SQRT(-POV3CU-QOV2SQ)/QOV2)                            LAP7 940
      IF(PHI)300,305,305                                                LAP7 950
  300 PHI=PHI+PI                                                        LAP7 960
  305 ROOT=2.0D0*DSQRT(-POV3)*DCOS(PHI/3.0D0)-AOV3                      LAP7 970
CS305 ROOT=2.0  * SQRT(-POV3)* COS(PHI/3.0  )-AOV3                      LAP7 980
      GO TO 325                                                         LAP7 990
C     ***** THREE REAL ROOTS, AT LEAST TWO ARE EQUAL *****              LAP71000
  310 ITYPE=2                                                           LAP71010
C     ***** CHECK SIGNS OF INVARIANTS A/3 AND B/3 *****                 LAP71020
      IF(AOV3)315,320,320                                               LAP71030
  315 IF(BOV3)420,320,320                                               LAP71040
C     ***** CALCULATE REPEATED RCOT OF CUBIC EQUATION *****             LAP71050
  320 ROOT=DSIGN(DSQRT(-POV3),QOV2)-AOV3                                LAP71060
CS320 ROOT= SIGN( SQRT(-POV3),QOV2)-AOV3                                LAP71070
C     ***** FORM DEGENERATE CONIC (LINE PAIR WHICH MAY BE COINCIDENT) **LAP71080
  325 DO 330 J=1,3                                                      LAP71090
      DO 330 K=1,3                                                      LAP71100
  330 DA(J,K)=QA(J,K,1)+ROOT*QA(J,K,2)                                  LAP71110
C     ***** EXAMINE INVARIANTS OF THE DEGENERATE CONIC *****            LAP71120
      T6=DA(1,1)*DA(2,2)                                                LAP71130
      T7=DA(1,2)**2                                                     LAP71140
C     ***** NEGATIVE DENOTES REAL INTERSECTING LINE PAIR *****          LAP71150
C     ***** POSITIVE DENOTES IMAGINARY LINES INTERSECTING AT REAL POINT LAP71160
      IF(T6-T7)335,345,340                                              LAP71170
  335 IF(T6*1.0001  -T7)400,345,345                                     LAP71180
  340 IF(T6-1.0001  *T7)345,345,365                                     LAP71190
  345 T8=DA(3,3)*(DA(1,1)+DA(2,2))                                      LAP71200
      T9=DA(1,3)**2+DA(2,3)**2                                          LAP71210
C     ***** NEGATIVE DENOTES REAL PARALLEL LINE PAIR *****              LAP71220
C     ***** POSITIVE DENOTES IMAGINARY PARALLELS *****                  LAP71230
C     ***** ZERO DENOTES ONE REAL LINE (COINCIDENT PARALLELS) *****     LAP71240
      IF(T8-T9)350,360,355                                              LAP71250
  350 IF(T8*1.0001  -T9)400,360,360                                     LAP71260
  355 IF(T8-1.0001  *T9)360,360,365                                     LAP71270
C     ***** COINCIDENT LINE PAIR FOUND FOR THE REPEATED ROOT *****      LAP71280
  360 ITYPE=3                                                           LAP71290
C     ***** COMPARE AREAS OF CONICS *****                               LAP71300
  365 KA=1                                                              LAP71310
      KB=2                                                              LAP71320
      IF(QC(3,3,KA)-QC(3,3,KB))370,375,375                              LAP71330
  370 KA=2                                                              LAP71340
      KB=1                                                              LAP71350
C     ***** SEE IF ONE CONIC IS INSIDE THE OTHER CONIC *****            LAP71360
  375 T1=0.0                                                            LAP71370
      DO 385 J=1,3                                                      LAP71380
      T2=QA(J,3,KB)                                                     LAP71390
      DO 380 K=1,2                                                      LAP71400
  380 T2=T2+QA(J,K,KB)*V12(K,KA)                                        LAP71410
  385 T1=T1+V12(J,KA)*T2                                                LAP71420
C     ***** DISCARD IF KA IS OUTSIDE KB *****                           LAP71430
      IF(T1)390,390,420                                                 LAP71440
  390 IF(KA-1)395,395,400                                               LAP71450
C     ***** THE OVERLAPPING ATOM HIDES THE ORIGINAL ATOM *****          LAP71460
  395 ICQ=-1                                                            LAP71470
      RETURN                                                            LAP71480
C     ***** STORE OVERLAPPING ATOM *****                                LAP71490
  400 ICQ=ICQ+1                                                         LAP71500
      IF(NCOVER-20)410,405,405                                          LAP71510
  405 NG=17                                                             LAP71520
      CALL ERPNT(ATOMS(1,IA),700)                                       LAP71530
      NCOVER=NCOVER-1                                                   LAP71540
  410 NCOVER=NCOVER+1                                                   LAP71550
      IJ=1                                                              LAP71560
      DO 415 I=1,3                                                      LAP71570
      DO 415 J=I,3                                                      LAP71580
      COVER(IJ,NCOVER)=QA(I,J,2)                                        LAP71590
  415 IJ=IJ+1                                                           LAP71600
      KC(NCOVER)=IA                                                     LAP71610
  420 CONTINUE                                                          LAP71620
C     ***** SECOND PART OF SUBROUTINE CHECKS FOR BONDS OVER THE ATOM ***LAP71630
  425 IF(NQUAD)470,470,430                                              LAP71640
  430 ITY=0                                                             LAP71650
C     ***** ROUGH CHECK FOR OVERLAPPING BONDS *****                     LAP71660
      DO 465 IQ=1,NQUAD                                                 LAP71670
      TID=QUAD(9,IQ)                                                    LAP71680
      NA1=TID/1000.                                                     LAP71690
      NA2=AMOD(TID,1000.)                                               LAP71700
      IF(NA-NA2)435,435,465                                             LAP71710
  435 DO 445 J=1,2                                                      LAP71720
      IF(YMAX(J)-AMIN1(QUAD(J,IQ),QUAD(J+2,IQ),QUAD(J+4,IQ),QUAD(J+6,IQ)LAP71730
     1 ))465,465,440                                                    LAP71740
  440 IF(YMIN(J)-AMAX1(QUAD(J,IQ),QUAD(J+2,IQ),QUAD(J+4,IQ),QUAD(J+6,IQ)LAP71750
     1 ))445,465,465                                                    LAP71760
  445 CONTINUE                                                          LAP71770
C     ***** EXACT CHECK FOR OVERLAPPING BONDS *****                     LAP71780
  450 ITY=ITY-1                                                         LAP71790
      IQQ=0                                                             LAP71800
      CALL LAPAB(IQ,NA,IQQ,ITY)                                         LAP71810
      IF(IQQ)455,460,460                                                LAP71820
  455 ICQ=-1                                                            LAP71830
      RETURN                                                            LAP71840
  460 ICQ=ICQ+1                                                         LAP71850
      IF(NQOVER-30)465,470,470                                          LAP71860
  465 CONTINUE                                                          LAP71870
  470 RETURN                                                            LAP71880
      END                                                               LAP71890


      SUBROUTINE LAP800(NA1,NA2,ICQ)                                    LAP8  10
C     ***** SUBROUTINE CHECKS FOR ATOMS AND BONDS OVERLAPPING A BOND ***LAP8  20
      DIMENSION FL(4,4),Y1(2),Y2(2),YMAX(2),YMIN(2),QUA(3,4)            LAP8  30
      DIMENSION VUE(3)                                                  LAP8  40
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER, LAP8  50
     1 NCOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)         LAP8  60
      REAL*8 CHEM                                                       LAP8  70
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    LAP8  80
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)LAP8  90
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) LAP8 100
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAP8 110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   LAP8 120
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   LAP8 130
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAP8 140
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      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   LAP8 150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD LAP8 160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REPV,RES,RMS,SCAL1LAP8 170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAP8 180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                LAP8 190
      IQ=0                                                              LAP8 200
      ICQ=0                                                             LAP8 210
      IF(NA1*NA2)245,245,195                                            LAP8 220
  195 TID1=FLOAT(NA1)*1000.+FLOAT(NA2)                                  LAP8 230
      IF(NCONIC)245,245,200                                             LAP8 240
  200 IF(NJ2-21)250,205,205                                             LAP8 250
C     ***** PART 1, CALLED FROM BOND, STORES BOND OUTLINE INFORMATION **LAP8 260
  205 IF(NQUAD-599)215,210,210                                          LAP8 270
  210 NG=16                                                             LAP8 280
      CALL ERPNT(ATOMS(1,NA1),822)                                      LAP8 290
      GO TO 245                                                         LAP8 300
  215 NQUAD=NQUAD+1                                                     LAP8 310
C     ***** CALCULATE OVERLAP MARGIN FOR BOND QUADRANGLE *****          LAP8 320
      T1=0.0                                                            LAP8 330
      T2=0.0                                                            LAP8 340
      DO 220 J=1,2                                                      LAP8 350
      Y1(J)=DP(J,1)-DP(J,65)                                            LAP8 360
      Y2(J)=DP(J,2)-DP(J,66)                                            LAP8 370
      T1=T1+Y1(J)**2                                                    LAP8 380
  220 T2=T2+Y2(J)**2                                                    LAP8 390
      IF(T1*T2)225,225,230                                              LAP8 400
  225 T1=0.0                                                            LAP8 410
      T2=0.0                                                            LAP8 420
      GO TO 235                                                         LAP8 430
  230 T1=OVMRGN/SQRT(T1)                                                LAP8 440
      T2=OVMRGN/SQRT(T2)                                                LAP8 450
C     ***** STORE BOND QUADRANGLE *****                                 LAP8 460
  235 DO 240 J=1,2                                                      LAP8 470
      Y1(J)=Y1(J)*T1                                                    LAP8 480
      Y2(J)=Y2(J)*T2                                                    LAP8 490
      QUAD(J,NQUAD)=DP(J,1)+Y1(J)                                       LAP8 500
      QUAD(J+2 ,NQUAD)=DP(J,2)+Y2(J)                                    LAP8 510
      QUAD(J+4,NQUAD)=DP(J,66)-Y2(J)                                    LAP8 520
  240 QUAD(J+6,NQUAD)=DP(J,65)-Y1(J)                                    LAP8 530
      QUAD(9,NQUAD)=TID1                                                LAP8 540
  245 RETURN                                                            LAP8 550
C     ***** PART 2, CALLED FROM BOND, OVERLAP CHECK FOR BOND NA1-NA2 ***LAP8 560
  250 NCOVER=0                                                          LAP8 570
      NQOVER=0                                                          LAP8 580
      TOL=1.E-5                                                         LAP8 590
      IF(NCONIC-NA1)245,245,255                                         LAP8 600
C     ***** SAVE QUADRANGLE TEMPORARILY *****                           LAP8 610
  255 IQ=NQUAD+1                                                        LAP8 620
      DO 260 J=1,2                                                      LAP8 630
      QUAD(J,IQ)=DP(J,1)                                                LAP8 640
      QUAD(J+2,IQ)=DP(J,2)                                              LAP8 650
      QUAD(J+4,IQ)=DP(J,66)                                             LAP8 660
  260 QUAD(J+6,IQ)=DP(J,65)                                             LAP8 670
      QUAD(9,IQ)=TID1                                                   LAP8 680
C     ***** FIT RECTANGLE AROUND QUADRANGLE *****                       LAP8 690
  265 DO 270 J=1,2                                                      LAP8 700
      YMIN(J)=AMIN1(DP(J,1),DP(J,2),DP(J,66),DP(J,65))                  LAP8 710
  270 YMAX(J)=AMAX1(DP(J,1),DP(J,2),DP(J,66),DP(J,65))                  LAP8 720
C     ***** ROUGH CHECK FOR ATOM-OVER-BOND OVERLAP *****                LAP8 730
      NA1P1=NA1+1                                                       LAP8 740
      ITY=0                                                             LAP8 750
      DO 305 IA=NA1P1,NCONIC                                            LAP8 760
      DO 285 J=1,2                                                      LAP8 770
      IF(IA-NA2)275,305,275                                             LAP8 780
  275 IF(YMAX(J)-CONIC(2*J-1,IA))305,305,280                            LAP8 790
  280 IF(YMIN(J)-CONIC(2*J,IA))285,305,305                              LAP8 800
  285 CONTINUE                                                          LAP8 810
C     ***** CHECK FOR TRUE ATOM-OVER-BOND OVERLAP *****                 LAP8 820
      ITY=ITY+1                                                         LAP8 830
      CALL LAPAB(IQ,IA,IQQ,ITY)                                         LAP8 840
      IF(IQQ)290,305,300                                                LAP8 850
C     ***** HIDDEN BOND *****                                           LAP8 860
  290 ICQ=-1                                                            LAP8 870
  295 RETURN                                                            LAP8 880
  300 ICQ=ICQ+1                                                         LAP8 890
      IF(NCOVER-20)305,310,310                                          LAP8 900
  305 CONTINUE                                                          LAP8 910
  310 IF(NQUAD)295,295,315                                              LAP8 920
C     ***** ROUGH CHECK FOR BOND-OVER-BOND OVERLAP *****                LAP8 930
  315 CALL DIFV(ATOMS(2,NA2),ATOMS(2,NA1),V1)                           LAP8 940
      CALL UNIT(V1,V1,1)                                                LAP8 950
      VUE(1)=  ATOMS(2,NA1)                                             LAP8 960
      VUE(2)=  ATOMS(3,NA1)                                             LAP8 970
      VUE(3)=  ATOMS(4,NA1)-VIEW                                        LAP8 980
      DO 495 IB=1,NQUAD                                                 LAP8 990
      TID2=QUAD(9,IB)                                                   LAP81000
      IF(TID1-TID2)320,495,320                                          LAP81010
  320 NB2=AMOD(TID2,1000.)                                              LAP81020
      NB1=TID2/1000.                                                    LAP81030
      IF(NA1-NB2)325,495,495                                            LAP81040
  325 DO 335 J=1,2                                                      LAP81050
      IF(YMAX(J)-AMIN1(QUAD(J,IB),QUAD(J+2,IB),QUAD(J+4,IB),QUAD(J+6,IB)LAP81060
     1 ))495,495,330                                                    LAP81070
  330 IF(YMIN(J)-AMAX1(QUAD(J,IB),QUAD(J+2,IB),QUAD(J+4,IB),QUAD(J+6,IB)LAP81080
     1 ))335,495,495                                                    LAP81090
  335 CONTINUE                                                          LAP81100
C     ***** SET UP LINEAR FORMS FOR EDGES OF QUADRANGLE *****           LAP81110
      DO 345 L=1,4                                                      LAP81120
      K=2*L                                                             LAP81130
      K1=MOD(K,8)+2                                                     LAP81140
      QUA(1,L)=QUAD(K,IB)-QUAD(K1,IB)                                   LAP81150
      QUA(2,L)=QUAD(K1-1,IB)-QUAD(K-1,IB)                               LAP81160
      QUA(3,L)=QUAD(K-1,IB)*QUAD(K1,IB)-QUAD(K,IB)*QUAD(K1-1,IB)        LAP81170
C     ***** NORMALIZE LINE EQUATION COEFFICIENTS *****                  LAP81180
      T1=SQRT(QUA(1,L)**2+QUA(2,L)**2)                                  LAP81190
      IF(T1)495,495,340                                                 LAP81200
  340 DO 345 J=1,3                                                      LAP81210
  345 QUA(J,L)=QUA(J,L)/T1                                              LAP81220
C     ***** EVALUATE LINEAR FORMS AND SIGNATURES FOR QUADRANGLE *****   LAP81230
      T3=3.0                                                            LAP81240
      DO 365 K=1,4                                                      LAP81250
      T2=3.0                                                            LAP81260
      J=K*2                                                             LAP81270
      DO 355 L=1,4                                                      LAP81280
      T1=QUAD(J-1,IQ)*QUA(1,L)+QUAD(J,IQ)*QUA(2,L)+QUA(3,L)             LAP81290
      IF(T1)350,355,355                                                 LAP81300
  350 T2=T2-1.0                                                         LAP81310
  355 FL(L,K)=T1                                                        LAP81320
      IF(T2)360,365,365                                                 LAP81330
  360 T3=T3-1.0                                                         LAP81340
  365 CONTINUE                                                          LAP81350
C     ***** CHECK FOR 4 POINTS INSIDE QUADRANGLE *****                  LAP81360
      IF(T3)370,375,375                                                 LAP81370
  370 ITYPE=-1                                                          LAP81380
      GO TO 415                                                         LAP81390
C     ***** CHECK FOR 1 TO 3 POINTS INSIDE QUADRANGLE ****              LAP81400
  375 IF(T3-3.0)380,385,385                                             LAP81410
  380 ITYPE=0                                                           LAP81420
      GO TO 415                                                         LAP81430
C     ***** DETERMINE WHICH EDGES ARE CROSSED BY THE 4 LINE SEGMENTS ***LAP81440
  385 DO 405 L=1,4                                                      LAP81450
      L1=MOD(L,4)+1                                                     LAP81460
C     ***** LINE SEGMENT L FROM POINT Y1 TO POINT Y2 *****              LAP81470
      Y1(1)=QUAD(L*2-1,IQ)                                              LAP81480
      Y1(2)=QUAD(L*2,IQ)                                                LAP81490
      Y2(1)=QUAD(L1*2-1,IQ)                                             LAP81500
      Y2(2)=QUAD(L1*2,IQ)                                               LAP81510
      DO 405 K=1,4                                                      LAP81520
      T1=FL(K,L)                                                        LAP81530
      T2=FL(K,L1)                                                       LAP81540
      T3=T1-T2                                                          LAP81550
C     ***** T1 AND T2 MUST HAVE OPPOSITE SIGNS FOR INTERSECTION TO OCCURLAP81560
      IF(T1*T2)390,390,405                                              LAP81570
C     ***** COMPONENT OF SEGMENT L PERPENDICULAR TO EDGE K OF IB IS T3  LAP81580
  390 IF(ABS(T3)-1.E-5)405,405,395                                      LAP81590
C     ***** CALCULATE COORDINATES OF INTERSECTION *****                 LAP81600
  395 T4=(T1*Y2(1)-T2*Y1(1))/T3                                         LAP81610
      T5=(T1*Y2(2)-T2*Y1(2))/T3                                         LAP81620
      K0=2*K                                                            LAP81630
      K1=2*(MOD(K,4)+1)                                                 LAP81640
C     ***** IS INTERSECTION WITHIN QUADRANGLE IQ *****                  LAP81650
      T6=(T4-QUAD(K0-1,IB))*(QUAD(K1-1,IB)-T4)+(T5-QUAD(K0,IB))*        LAP81660
     1 (QUAD(K1,IB)-T5)                                                 LAP81670
      IF(ABS(T6)-1.E-4)410,410,400                                      LAP81680
  400 IF(T6)405,410,410                                                 LAP81690
  405 CONTINUE                                                          LAP81700
      GO TO 495                                                         LAP81710
  410 ITYPE=1                                                           LAP81720
C     ***** CHECK OVER/UNDER AMBIGUITY *****                            LAP81730
  415 IF((NA1-NB1)*(NA2-NB2)*(NA2-NB1))425,420,425                      LAP81740
C     ***** BONDS SHARE AN ATOM *****                                   LAP81750
  420 IF(NA1+NA2-NB1-NB2)465,495,495                                    LAP81760
  425 CALL DIFV(ATOMS(2,NB2),ATOMS(2,NB1),V2)                           LAP81770
      CALL DIFV(ATOMS(2,NB1),ATOMS(2,NA1),V4)                           LAP81780
      CALL UNIT(V2,V2,1)                                                LAP81790
      CALL UNIT(V4,V4,1)                                                LAP81800
      CALL NORM(V1,V2,V3,1)                                             LAP81810
      IF(VV(V3,V3)-TOL)430,430,435                                      LAP81820
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C     ***** PARALLEL BONDS, RECALCULATE V3 *****                        LAP81830
  430 CALL NORM(V1,V4,V5,1)                                              LAP81840
      CALL NORM(V5,V1,V3,1)                                              LAP81850
C     ***** CHECK FOR COLLINEAR BONDS *****                              LAP81860
      IF(VV(V3,V3)-TOL)465,465,450                                       LAP81870
  435 IF(VV(V3,V4)+TOL)440,450,450                                       LAP81880
  440 DO 445 J=1,3                                                       LAP81890
  445 V3(J)=-V3(J)                                                       LAP81900
C     ***** V3 IS NORMAL TO BONDS IQ AND IB GOING FROM IQ TOWARD IB ***  LAP81910
  450 IF(VIEW)455,455,460                                                LAP81920
  455 IF(V3(3))495,495,465                                               LAP81930
  460 IF(VV(VUE,V3))465,495,495                                          LAP81940
C     ***** OVERLAPPING BOND FOUND *****                                 LAP81950
  465 ICQ=ICQ+1                                                          LAP81960
      IF(ITYPE)470,475,475                                               LAP81970
C     ***** HIDDEN BOND *****                                            LAP81980
  470 ICQ=-1                                                             LAP81990
      RETURN                                                             LAP82000
C     ***** STORE INTERFERING QUADRANGLE *****                           LAP82010
  475 IF(NQOVER-30)485,480,480                                           LAP82020
  480 NG=17                                                              LAP82030
      CALL ERPNT(TID2,800)                                               LAP82040
      RETURN                                                             LAP82050
  485 NQOVER=NQOVER+1                                                    LAP82060
      DO 490 K=1,4                                                       LAP82070
      DO 490 J=1,3                                                       LAP82080
  490 QOVER(J,K,NQOVER)=QUA(J,K)                                         LAP82090
      KQ(NQOVER)=IB                                                      LAP82100
  495 CONTINUE                                                           LAP82110
  500 RETURN                                                             LAP82120
      END                                                                LAP82130


      SUBROUTINE LAPAB(IQ,IA,ICQ,ITY)                                    LAPA  10
C     ***** SUBROUTINE CHECKS FOR OVERLAP BETWEEN ATOMS AND BONDS *****  LAPA  20
C     ***** CALLED BY SUBROUTINES LAP700 AND LAP800 *****                LAPA  30
      DIMENSION BF(4),CON(3,3),QF(5),QUA(3,4)                            LAPA  40
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER,  LAPA  50
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)          LAPA  60
      REAL*8 CHEM                                                        LAPA  70
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)     LAPA  80
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) LAPA  90
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)  LAPA 100
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  LAPA 110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)    LAPA 120
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    LAPA 130
      DIMENSION XLNG(3),XO(3),XT(3)                                      LAPA 140
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D    LAPA 150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,IATM,LINO,NATOM,NCD  LAPA 160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAPA 170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    LAPA 180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                 LAPA 190
      TID=QUAD(9,IQ)                                                     LAPA 200
      NA1=TID/1000.                                                      LAPA 210
      NA2=AMOD(TID,1000.)                                                LAPA 220
C     ***** ITY.GT.0, CHECK FOR ATOMS OVER A BOND ****                   LAPA 230
C     ***** ITY.LT.0, CHECK FOR BONDS OVER AN ATOM *****                 LAPA 240
      ICQ=0                                                              LAPA 250
      IF(ITY)210,200,205                                                 LAPA 260
  200 RETURN                                                             LAPA 270
  205 CALL LAPCON(CONIC(1,IA),CON,V1,0.0)                                LAPA 280
      IF(ITY-2)220,240,240                                               LAPA 290
  210 IF(ITY+2)220,220,215                                               LAPA 300
  215 CALL LAPCON(CONIC(1,IA),CON,V1,OVMRGN)                             LAPA 310
C     ***** SET UP LINEAR FORMS FOR EDGES OF QUADRANGLE *****            LAPA 320
  220 DO 235 L=1,4                                                       LAPA 330
      K=2*L                                                              LAPA 340
      K1=MOD(K,8)+2                                                      LAPA 350
      QUA(1,L)=QUAD(K,IQ)-QUAD(K1,IQ)                                    LAPA 360
      QUA(2,L)=QUAD(K1-1,IQ)-QUAD(K-1,IQ)                                LAPA 370
      QUA(3,L)=QUAD(K-1,IQ)*QUAD(K1,IQ)-QUAD(K,IQ)*QUAD(K1-1,IQ)         LAPA 380
      T1=SQRT(QUA(1,L)**2+QUA(2,L)**2)                                   LAPA 390
      IF(T1)225,225,230                                                  LAPA 400
  225 ITY=0                                                              LAPA 410
      ICQ=0                                                              LAPA 420
      GO TO 430                                                          LAPA 430
C     ***** TRANSFORM COEFFICIENTS FOR EDGES TO NORMAL FORM *****        LAPA 440
  230 DO 235 J=1,3                                                       LAPA 450
  235 QUA(J,L)=QUA(J,L)/T1                                               LAPA 460
C     ***** EVALUATE 4 QUADRATIC AND 4 BILINEAR FORMS *****              LAPA 470
  240 V2(3)=1.0                                                          LAPA 480
      V3(3)=1.0                                                          LAPA 490
      T2=3.0                                                             LAPA 500
      DO 265 L=1,4                                                       LAPA 510
      L1=(MOD(L,4)+1)*2                                                  LAPA 520
      V2(1)=QUAD(2*L-1,IQ)                                               LAPA 530
      V2(2)=QUAD(2*L,IQ)                                                 LAPA 540
      V3(1)=QUAD(L1-1,IQ)                                                LAPA 550
      V3(2)=QUAD(L1,IQ)                                                  LAPA 560
      QF(L)=0.0                                                          LAPA 570
      BF(L)=0.0                                                          LAPA 580
      DO 250 K=1,3                                                       LAPA 590
      T1=CON(3,K)                                                        LAPA 600
      DO 245 J=1,2                                                       LAPA 610
  245 T1=T1+V2(J)*CON(J,K)                                               LAPA 620
      QF(L)=QF(L)+T1*V2(K)                                               LAPA 630
  250 BF(L)=BF(L)+T1*V3(K)                                               LAPA 640
      IF(QF(L))260,255,265                                               LAPA 650
  255 T2=T2-0.8                                                          LAPA 660
      GO TO 265                                                          LAPA 670
  260 T2=T2-1.0                                                          LAPA 680
  265 CONTINUE                                                           LAPA 690
      QF(5)=QF(1)                                                        LAPA 700
C     ***** CHECK FOR 4 POINTS OF QUADRANGLE INSIDE OR ON ELLIPSE ***** LAPA 710
      IF(T2)270,275,275                                                  LAPA 720
  270 ITYPE=-1                                                           LAPA 730
      GO TO 330                                                          LAPA 740
C     ***** CHECK FOR 1 TO 3 POINTS OF QUADRANGLE INSIDE THE ELLIPSE ***LAPA 750
  275 IF(T2-2.2)280,285,285                                              LAPA 760
  280 ITYPE=0                                                            LAPA 770
      IF(NA2-IA)340,375,335                                              LAPA 780
C     ***** CHECK FOR QUADRANGLE-ELLIPSE INTERSECTION *****              LAPA 790
  285 DO 305 K=1,4                                                       LAPA 800
C     ***** EVALUATE DISCRIMINANT *****                                  LAPA 810
      T1=BF(K)**2-QF(K)*QF(K+1)                                          LAPA 820
      IF(T1)305,305,290                                                  LAPA 830
  290 T1=SQRT(T1)                                                        LAPA 840
C     ***** IS INTERSECTION WITHIN BOUNDS OF QUADRANGLE *****            LAPA 850
      T3=QF(K)-BF(K)                                                     LAPA 860
      T4=T3+QF(K+1)-BF(K)                                                LAPA 870
      IF(ABS(T4)-1.E-5)305,305,295                                       LAPA 880
  295 T5=(T3-T1)/T4                                                      LAPA 890
      IF(T5)305,280,300                                                  LAPA 900
  300 IF(1.0-T5)305,305,280                                              LAPA 910
  305 CONTINUE                                                           LAPA 920
C     ***** NO VALID INTERSECTION FOUND *****                            LAPA 930
C     ***** CHECK FOR CENTER OF ELLIPSE WITHIN THE QUADRANGLE ****       LAPA 940
      T3=3.0                                                             LAPA 950
      DO 320 K=1,4                                                       LAPA 960
      T1=QUA(3,K)                                                        LAPA 970
      DO 310 J=1,2                                                       LAPA 980
  310 T1=T1+V1(J)*QUA(J,K)                                               LAPA 990
      IF(T1)315,320,320                                                  LAPA1000
  315 T3=T3-1.0                                                          LAPA1010
  320 CONTINUE                                                           LAPA1020
      IF(T3)325,370,370                                                  LAPA1030
  325 ITYPE=1                                                            LAPA1040
C     ***** CHECK OVER/UNDER AMBIGUITY *****                             LAPA1050
  330 IF(NA2-IA)375,375,335                                              LAPA1060
  335 IF(IA-NA1)375,375,340                                              LAPA1070
  340 CALL DIFV(ATOMS(2,NA2),ATOMS(2,NA1),V2)                            LAPA1080
      CALL DIFV(ATOMS(2,IA),ATOMS(2,NA1),V3)                             LAPA1090
      CALL UNIT(V2,V2,1)                                                 LAPA1100
      CALL UNIT(V3,V3,1)                                                 LAPA1110
      CALL NORM(V2,V3,V4,1)                                              LAPA1120
      IF(VV(V4,V4)-1.E-5)345,345,350                                     LAPA1130
C     ***** CENTER OF ATOM IQ IS ON THE BOND LINE *****                  LAPA1140
  345 IF(ITY)370,370,385                                                 LAPA1150
C     ***** CENTER OF ATOM IQ IS NOT ON THE BOND LINE *****              LAPA1160
  350 CALL NORM(V4,V2,V5,1)                                              LAPA1170
      T1=-V5(3)                                                          LAPA1180
      IF(VIEW)365,365,355                                                LAPA1190
  355 T1=V5(3)*(ATOMS(4,IA)-VIEW)                                        LAPA1200
      DO 360 J=1,2                                                       LAPA1210
  360 T1=T1+V5(J)*ATOMS(J+1,IA)                                          LAPA1220
  365 IF(T1*FLOAT(ITY))375,375,370                                       LAPA1230
C     ***** NO INTERFERENCE FOUND *****                                  LAPA1240
  370 ICQ=0                                                              LAPA1250
      GO TO 430                                                          LAPA1260
C     ***** ITYPE=1 ENCLOSED ELLIPSE / ITYPE=-1 ENCLOSED QUADRANGLE ****LAPA1270
  375 IF(ITYPE*ITY)380,385,385                                           LAPA1280
C     ***** HIDDEN ATOM OR HIDDEN BOND *****                             LAPA1290
  380 ICQ=-1                                                             LAPA1300
      GO TO 430                                                          LAPA1310
  385 ICQ=1                                                              LAPA1320
      IF(ITY)410,390,390                                                 LAPA1330
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C     ***** STORE INTERFERING ELLIPSE *****                              LAPA1340
  390 IF(NCOVER-20)400,395,395                                            LAPA1350
  395 NG=17                                                               LAPA1360
      CALL ERPNT(ATOMS(1,IA),800)                                         LAPA1370
      NCOVER=NCOVER-1                                                     LAPA1380
  400 NCOVER=NCOVER+1                                                     LAPA1390
      IJ=1                                                                LAPA1400
      DO 405 I=1,3                                                        LAPA1410
      DO 405 J=I,3                                                        LAPA1420
      COVER(IJ,NCOVER)=CON(I,J)                                           LAPA1430
  405 IJ=IJ+1                                                             LAPA1440
      KC(NCOVER)=IA                                                       LAPA1450
      GO TO 430                                                           LAPA1460
C     ***** STORE INTERFERING QUADRANGLE *****                            LAPA1470
  410 IF(NQOVER-30)420,415,415                                            LAPA1480
  415 NG=18                                                               LAPA1490
      CALL ERPNT(TID,700)                                                 LAPA1500
      NQOVER=NQOVER-1                                                     LAPA1510
  420 NQOVER=NQOVER+1                                                     LAPA1520
      DO 425 K=1,4                                                        LAPA1530
      DO 425 J=1,3                                                        LAPA1540
  425 QOVER(J,K,NQOVER)=QUA(J,K)                                          LAPA1550
      KQ(NQOVER)=IQ                                                       LAPA1560
  430 RETURN                                                              LAPA1570
      END                                                                 LAPA1580


      SUBROUTINE LAPCON(CON1,CON,Y,OVMR)                                  LAPC  10
C     ***** TRANSFORM CONIC TO PLOTTER HOMOGENEOUS COORDINATE SYSTEM ***LAPC  20
C     ***** CALLED BY SUBROUTINES LAP700 AND LAPAB *****                  LAPC  30
      DIMENSION CON1(7),CON(3,3),Y(3)                                     LAPC  40
      Y(1)=(CON1(1)+CON1(2))*0.5                                          LAPC  50
      Y(2)=(CON1(3)+CON1(4))*0.5                                          LAPC  60
      Y(3)=1.0                                                            LAPC  70
      CON(1,1)=CON1(5)                                                    LAPC  80
      CON(1,2)=CON1(6)                                                    LAPC  90
      CON(2,1)=CON1(6)                                                    LAPC 100
      CON(2,2)=CON1(7)                                                    LAPC 110
      T1=(CON1(2)-CON1(1)+CON1(4)-CON1(3))*0.25                           LAPC 120
      CON(3,3)=-((T1-OVMR)/T1)**2                                         LAPC 130
      DO 205 K=1,2                                                        LAPC 140
      CON(K,3)=0.0                                                        LAPC 150
      DO 200 J=1,2                                                        LAPC 160
  200 CON(K,3)=CON(K,3)-Y(J)*CON(J,K)                                     LAPC 170
      CON(3,K)=CON(K,3)                                                   LAPC 180
  205 CON(3,3)=CON(3,3)-CON(3,K)*Y(K)                                     LAPC 190
      RETURN                                                              LAPC 200
      END                                                                 LAPC 210


      SUBROUTINE LAPDRW(Y,NPEN,NCQ)                                       LAPD  10
C     ***** SUBROUTINE ELIMINATES HIDDEN LINES AND DRAWS VISIBLE LINES *LAPD  20
      DIMENSION CB(20),CQ(50,2),QL(4,30,2),SEG(2),Y(3),YN(3),YO(3),Z(3) LAPD  30
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER, LAPD  40
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)          LAPD  50
      REAL*8 CHEM                                                         LAPD  60
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      LAPD  70
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) LAPD  80
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) LAPD  90
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAPD 100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   LAPD 110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   LAPD 120
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAPD 130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   LAPD 140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,IATM,LTNO,NATOM,NCD LAPD 150
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAPD 160
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAPD 170
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                LAPD 180
      NCQ=NCOVER+NQOVER                                                 LAPD 190
      IF(NCQ)200,200,205                                                LAPD 200
  200 RETURN                                                            LAPD 210
C     ***** CHECK ALL OVERLAPPING ATOMS AND BONDS *****                 LAPD 220
  205 NPM3=NPEN-3                                                       LAPD 230
      IF(NPM3)  210,230,230                                             LAPD 240
C     ***** SAVE INFORMATION FROM LAST POINT IF PEN IS DOWN *****       LAPD 250
  210 YO(1)=YN(1)                                                       LAPD 260
      YO(2)=YN(2)                                                       LAPD 270
      YO(3)=1.0                                                         LAPD 280
      NPO=NPN                                                           LAPD 290
      DO 215 K=1,NCQ                                                    LAPD 300
  215 CQ(K,1)=CQ(K,2)                                                   LAPD 310
      IF(NQOVER)230,230,220                                             LAPD 320
  220 DO 225 K=1,NQOVER                                                 LAPD 330
      DO 225 J=1,4                                                      LAPD 340
  225 QL(J,K,1)=QL(J,K,2)                                               LAPD 350
C     ***** EVALUATE CONIC QUADRATIC FORMS AT NEW POINT YN *****        LAPD 360
  230 YN(1)=Y(1)                                                        LAPD 370
      YN(2)=Y(2)                                                        LAPD 380
      YN(3)=1.0                                                         LAPD 390
      NPN=NPEN                                                          LAPD 400
      IF(NCOVER)250,250,235                                             LAPD 410
  235 DO 245 K=1,NCOVER                                                 LAPD 420
      Z(1)=YN(1)*COVER(1,K)+YN(2)*COVER(2,K)+COVER(3,K)                 LAPD 430
      Z(2)=YN(1)*COVER(2,K)+YN(2)*COVER(4,K)+COVER(5,K)                 LAPD 440
      Z(3)=YN(1)*COVER(3,K)+YN(2)*COVER(5,K)+COVER(6,K)                 LAPD 450
      CQ(K,2)=Z(1)*YN(1)+Z(2)*YN(2)+Z(3)                                LAPD 460
C     ***** EVALUATE CONIC BILINEAR FORM IF PEN IS DOWN *****           LAPD 470
      IF(NPM3)240,245,245                                               LAPD 480
  240 CB(K)= Z(1)*YO(1)+Z(2)*YO(2)+Z(3)                                 LAPD 490
  245 CONTINUE                                                          LAPD 500
C     ***** EVALUATE LINEAR FORMS AND SIGNATURE FOR QUADRANGLE *****    LAPD 510
  250 IF(NQOVER)275,275,255                                             LAPD 520
  255 KCQ=NCOVER                                                        LAPD 530
      DO 270 K=1,NQOVER                                                 LAPD 540
      T2=3.0                                                            LAPD 550
      DO 265 J=1,4                                                      LAPD 560
      T1=YN(1)*QOVER(1,J,K)+YN(2)*QOVER(2,J,K)+QOVER(3,J,K)             LAPD 570
      IF(T1)260,265,265                                                 LAPD 580
  260 T2=T2-1.0                                                         LAPD 590
  265 QL(J,K,2)=T1                                                      LAPD 600
      KCQ=KCQ+1                                                         LAPD 610
C     ***** T2=-1 INSIDE, =0 ACROSS ANY EDGE, =1 ACROSS ANY VERTEX *****LAPD 620
  270 CQ(KCQ,2)=T2                                                      LAPD 630
C     ***** IF PEN IS UP, OMIT ALL SUBSEQUENT CHECKING *****            LAPD 640
  275 IF(NPM3)285,280,280                                               LAPD 650
  280 NPN=3                                                             LAPD 660
      CALL SCRIBE(YN,NPN,LTNC)                                          LAPD 670
      RETURN                                                            LAPD 680
C     ***** CHECK FOR HIDDEN SEGMENT *****                              LAPD 690
  285 DO 295 K=1,NCQ                                                    LAPD 700
      IF(CQ(K,1))290,295,295                                            LAPD 710
  290 IF(CQ(K,2))280,295,295                                            LAPD 720
  295 CONTINUE                                                          LAPD 730
C     ***** FIND ENTRY AND EXIT POINTS ON EACH CONIC *****              LAPD 740
      NINT=0                                                            LAPD 750
      IF(NCOVER)330,330,300                                             LAPD 760
  300 DO 325 K=1,NCOVER                                                 LAPD 770
C     ***** EVALUATE DISCRIMINANT *****                                 LAPD 780
      T1=CB(K)**2-CQ(K,1)*CQ(K,2)                                       LAPD 790
      IF(T1)325,325,305                                                 LAPD 800
  305 T1=SQRT(T1)                                                       LAPD 810
C     ***** SOLVE QUADRATIC EQATION *****                               LAPD 820
      T2=CQ(K,1)-CB(K)                                                  LAPD 830
      T3=T2+CQ(K,2)-CB(K)                                               LAPD 840
      IF(ABS(T3)-1.E-5)325,325,310                                      LAPD 850
  310 T4=(T2-T1)/T3                                                     LAPD 860
      T5=(T2+T1)/T3                                                     LAPD 870
C     ***** VALID INTERSECTION IF T4.LT.1 AND T5.GT.0 *****             LAPD 880
      IF(T4-1.0)315,325,325                                             LAPD 890
  315 IF(T5)325,325,320                                                 LAPD 900
C     ***** SAVE VALID CONIC INTERSECTIONS *****                        LAPD 910
  320 NINT=NINT+1                                                       LAPD 920
      SEGM(NINT,1)=T4                                                   LAPD 930
      SEGM(NINT,2)=T5                                                   LAPD 940
  325 CONTINUE                                                          LAPD 950
  330 IF(NQOVER)425,425,335                                             LAPD 960
C     ***** FIND ENTRY AND EXIT POINTS FOR EACH QUADRANGLE *****        LAPD 970
  335 DO 420 K=1,NQOVER                                                 LAPD 980
      I12=0                                                             LAPD 990
      KCQ=NCOVER+K                                                      LAPD1000
C     ***** CHECK FOR SINGLE INSIDE POINT *****                         LAPD1010
      SEG(1)=CQ(KCQ,1)                                                  LAPD1020
      IF(SEG(1))345,340,340                                             LAPD1030
  340 SEG(1)=1.0-CQ(KCQ,2)                                              LAPD1040
      IF(SEG(1)-1.0)350,350,345                                         LAPD1050
C     ***** INSIDE POINT FOUND, ONLY ONE INTERSECTION POSSIBLE *****    LAPD1060
  345 I12=1                                                             LAPD1070
C     ***** FIND WHICH EDGES ARE CROSSED BY THE SEGMENT *****           LAPD1080
  350 DO 410 J=1,4                                                      LAPD1090
      T1=QL(J,K,1)                                                      LAPD1100
      T2=QL(J,K,2)                                                      LAPD1110
      T3=T1-T2                                                          LAPD1120
      IF(T1*T2)355,355,410                                              LAPD1130
C     ***** CHECK FOR SEGMENT ON AN EDGE *****                          LAPD1140
  355 IF(ABS(T3)-1.E-5)420,420,360                                      LAPD1150
C     ***** CALCULATE COORDINATES OF INTERSECTION *****                 LAPD1160
  360 T4=(T1*YN(1)-T2*YO(1))/T3                                         LAPD1170
      T5=(T1*YN(2)-T2*YO(2))/T3                                         LAPD1180
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      J1=2*(MOD(J,4)+1)                                                 LAPD1190
      IQ=KQ(K)                                                          LAPD1200
C     ***** IS INTERSECTION WITHIN LIMITS OF QUADRANGLE *****           LAPD1210
      T6=(T4-QUAD(2*J-1,IQ))*(QUAD(J1-1,IQ)-T4)+(T5-QUAD(2*J,IQ))*      LAPD1220
     1 (QUAD(J1,IQ)-T5)                                                 LAPD1230
      IF(ABS(T6)-1.E-4)370,370,365                                      LAPD1240
  365 IF(T6)410,370,370                                                 LAPD1250
C     ***** CALCULATE FRACTION PARAMETER AND STORE IT *****             LAPD1260
  370 T1=T1/T3                                                          LAPD1270
      IF(I12-1)375,380,395                                              LAPD1280
C     ***** STORE FIRST INTERSECTION *****                              LAPD1290
  375 I12=1                                                             LAPD1300
      GO TO 390                                                         LAPD1310
C     ***** STORE SECOND INTERSECTION ****                              LAPD1320
  380 I12=2                                                             LAPD1330
      IF(T1-SEG(1))385,405,405                                          LAPD1340
  385 SEG(2)=SEG(1)                                                     LAPD1350
  390 SEG(1)= T1                                                        LAPD1360
      GO TO 410                                                         LAPD1370
C     ***** MORE THAN TWO INTERSECTIONS (I.E.,QUADRANGLE DIAGONAL) *****LAPD1380
  395 IF(T1-SEG(1))390,410,400                                          LAPD1390
  400 IF(T1-SEG(2))410,410,405                                          LAPD1400
  405 SEG(2)=T1                                                         LAPD1410
  410 CONTINUE                                                          LAPD1420
      IF(I12-1)420,420,415                                              LAPD1430
C     ***** STORE FRACTION PARAMETERS *****                             LAPD1440
  415 NINT=NINT+1                                                       LAPD1450
      SEGM(NINT,1)=SEG(1)                                               LAPD1460
      SEGM(NINT,2)=SEG(2)                                               LAPD1470
  420 CONTINUE                                                          LAPD1480
C     ***** END OF ENTRY-AND-EXIT-POINT CALCULATIONS *****              LAPD1490
  425 IF(NINT-1)430,490,435                                             LAPD1500
C     ***** NO INTERFERENCE FOUND, DRAW ENTIRE SEGMENT *****            LAPD1510
  430 CALL SCRIBE(YN,2,LTNO)                                            LAPD1520
      RETURN                                                            LAPD1530
C     **** SORT SEGMENT INTERSECTION LIST *****                         LAPD1540
C     ***** SORTING PROCEDURE BY SHELL,D.L. COMM. ACM 2,30-32 (1959) ***LAPD1550
  435 M=NINT                                                            LAPD1560
  440 M=M/2                                                             LAPD1570
      IF(M)490,490,445                                                  LAPD1580
  445 K=NINT-M                                                          LAPD1590
      J=1                                                               LAPD1600
  450 I=J                                                               LAPD1610
  455 IM=I+M                                                            LAPD1620
      IF(SEGM(I,1))460,470,470                                          LAPD1630
  460 IF(SEGM(IM,1))465,465,485                                         LAPD1640
  465 IF(SEGM(I,2)-SEGM(IM,2))485,485,475                               LAPD1650
  470 IF(SEGM(I,1)-SEGM(IM,1))485,485,475                               LAPD1660
  475 DO 480 L=1,2                                                      LAPD1670
      T1=SEGM(I,L)                                                      LAPD1680
      SEGM(I,L)=SEGM(IM,L)                                              LAPD1690
  480 SEGM(IM,L)=T1                                                     LAPD1700
      I=I-M                                                             LAPD1710
      IF(I)485,485,455                                                  LAPD1720
  485 J=J+1                                                             LAPD1730
      IF(J-K)450,450,440                                                LAPD1740
C     ***** FIND STARTING POINT P0 AND END POINT P1 *****               LAPD1750
  490 P0=0.0                                                            LAPD1760
      K=0                                                               LAPD1770
  495 K=K+1                                                             LAPD1780
      IF(K-NINT)500,500,515                                             LAPD1790
  500 P1=SEGM(K,1)                                                      LAPD1800
      IF(P1)510,505,505                                                 LAPD1810
  505 IF(P1-P0)510,510,520                                              LAPD1820
  510 P0=AMAX1(P0,SEGM(K,2))                                            LAPD1830
      IF(P0-1.0)495,530,525                                             LAPD1840
  515 P1=1.0                                                            LAPD1850
C     ***** DRAW SEGMENT FROM P0 TO P1 *****                            LAPD1860
  520 IF(P0)535,535,530                                                 LAPD1870
  525 P0=1.0                                                            LAPD1880
  530 Z(1)=YO(1)*(1.-P0)+YN(1)*P0                                       LAPD1890
      Z(2)=YO(2)*(1.-P0)+YN(2)*P0                                       LAPD1900
      NPN=3                                                             LAPD1910
      CALL SCRIBE(Z,NPN,LTNO)                                           LAPD1920
      IF(P0-1.0)535,540,540                                             LAPD1930
  535 Z(1)=YO(1)*(1.-P1)+YN(1)*P1                                       LAPD1940
      Z(2)=YO(2)*(1.-P1)+YN(2)*P1                                       LAPD1950
      NPN=2                                                             LAPD1960
      CALL SCRIBE(Z,NPN,LTNO)                                           LAPD1970
      IF(P1-1.0)510,540,540                                             LAPD1980
  540 RETURN                                                            LAPD1990
      END                                                               LAPD2000
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      SUBROUTINE MM(X,Y,Z)                                              MM     10
C     MULTIPLY TWO MATRICES                                             MM     20
C     Z(3,3)=X(3,3)*Y(3,3)                                              MM     30
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                    MM     40
      DO 117 I=1,3                                                      MM     50
      DO 117 K=1,3                                                      MM     60
      Z(I,K)=0.0                                                        MM     70
      DO 117 J=1,3                                                      MM     80
  117 Z(I,K)=Z(I,K)+X(I,J)*Y(J,K)                                       MM     90
      RETURN                                                            MM    100
      END                                                               MM    110


      SUBROUTINE MV(X,Y,Z)                                              MV     10
C     MATRIX * VECTOR                                                   MV     20
C     Z(3)=X(3,3)*Y(3)                                                  MV     30
      DIMENSION X(3,3),Y(3),Z(3)                                        MV     40
      DO 113 I=1,3                                                      MV     50
      Z(I)=0.0                                                          MV     60
      DO 113 J=1,3                                                      MV     70
  113 Z(I)=Z(I)+X(I,J)*Y(J)                                             MV     80
      RETURN                                                            MV     90
      END                                                               MV    100


      SUBROUTINE NORM(X,Y,Z,ITYPE)                                      NORM   10
C     ***** VECTOR PRODUCT  Z=X*Y *****                                 NORM   20
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         NORM   30
      DIMENSION X(3),Y(3),Z(3),Z1(3)                                    NORM   40
      REAL*8 CHEM                                                       NORM   50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    NORM   60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)NORM   70
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) NORM   80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) NORM   90
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   NORM  100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   NORM  110
      DIMENSION XLNG(3),XO(3),XT(3)                                     NORM  120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   NORM  130
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD NORM  140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALINORM  150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   NORM  160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                NORM  170
      DO 125 J=1,3                                                      NORM  180
      I1=MOD(I+3,3)+1                                                   NORM  190
      I2=MOD(I+1,3)+1                                                   NORM  200
      T1=X(I1)*Y(I2)-X(I2)*Y(I1)                                        NORM  210
      IF(ITYPE)115,115,105                                              NORM  220
  105 Z(I)=T1                                                           NORM  230
      GO TO 125                                                         NORM  240
  115 Z1(I)=T1                                                          NORM  250
  125 CONTINUE                                                          NORM  260
      IF(ITYPE)135,135,300                                              NORM  270
  135 CALL MV(BB,Z1,Z)                                                  NORM  280
  300 RETURN                                                            NORM  290
      END                                                               NORM  300


      SUBROUTINE PAXES(ACODE,ITYPE)                                     PAXE   10
C     ***** ITYPE .LT.0 FOR COVARIANCE MATRIX IN Q *****                PAXE   20
C     ***** ITYPE .GT.0 FOR ELLIPSOID QUADRATIC FORM IN Q *****         PAXE   30
C     ***** XABSF(ITYPE)=1 BASED ON TRICLINIC COORDINATE SYSTEM *****   PAXE   40
C     ***** =2 OR 3 FOR WORKING OR REFERENCE CARTESIAN SYSTEMS *****    PAXE   50
C     ***** CONTRAVARIANT EIGENVECTORS FOR Q IN COLUMNS OF PAC *****    PAXE   60
C     ***** CHECK ATOM CODE *****                                       PAXE   70
      DIMENSION W(3,3),X(3)                                             PAXE   80
      REAL*8 CHEM                                                       PAXE   90
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PAXE  100
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)PAXE  110
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PAXE  120
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PAXE  130
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PAXE  140
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PAXE  150
      DIMENSION XLNG(3),XO(3),XT(3)                                     PAXE  160
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PAXE  170
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PAXE  180
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPAXE  190
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PAXE  200
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PAXE  210
      IT=IABS(ITYPE)-1                                                  PAXE  220
      KS=AMOD(ACODE,100.)                                               PAXE  230
      IF(NSYM-KS)105,115,115                                            PAXE  240
  105 NG=4                                                              PAXE  250
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      GO TO 300                                                         PAXE 260
  115 II=ACODE/100000.                                                  PAXE 270
      IF(NATOM-II) 125,130,130                                          PAXE 280
  125 NG=5                                                              PAXE 290
      GO TO 300                                                         PAXE 300
  130 IF(II) 125,125,135                                                PAXE 310
C     ***** CRYSTALLOGRAPHIC SYMMETRY ROTATION *****                    PAXE 320
  135 CALL TMM(PA(1,1,II),PS(1,1,KS),PAT)                               PAXE 330
      IF(IT-1) 160,145,155                                              PAXE 340
C     ***** TRANSFORM TO CARTESIAN SYSTEMS *****                        PAXE 350
  145 CALL TMM(PAT,AAWRK,PAC)                                           PAXE 360
      GO TO 175                                                         PAXE 370
  155 CALL TMM(PAT,AAREV,PAC)                                           PAXE 380
      GO TO 175                                                         PAXE 390
  160 IF(ITYPE) 162,155,170                                             PAXE 400
C     ***** TRANSFORM TO TRICLINIC SYSTEM *****                         PAXE 410
  162 DO 165 J=1,9                                                      PAXE 420
  165 PAC(J,1)=PAT(J,1)                                                 PAXE 430
      GO TO 175                                                         PAXE 440
  170 CALL MM(AA,PAT,PAC)                                               PAXE 450
C     ***** FORM DIAGONAL MATRIX OR ITS INVERSE *****                   PAXE 460
  175 DO 205 J=1,3                                                      PAXE 470
      T1=EV(J,II)                                                       PAXE 480
      IF(ITYPE) 195,195,185                                             PAXE 490
  185 X(J)=1./(T1*T1)                                                   PAXE 500
      GO TO 205                                                         PAXE 510
  195 X(J)=T1*T1                                                        PAXE 520
  205 RMS(J)=T1                                                         PAXE 530
C     ***** FORM QUADRATIC FORM *****                                   PAXE 540
      DO 245 I=1,3                                                      PAXE 550
      DO 245 J=I,3                                                      PAXE 560
      T1=0.0                                                            PAXE 570
      DO 225 K=1,3                                                      PAXE 580
  225 T1=T1+PAC(I,K)*PAC(J,K)*X(K)                                      PAXE 590
      Q(J,I)=T1                                                         PAXE 600
  245 Q(I,J)=T1                                                         PAXE 610
  300 RETURN                                                            PAXE 620
      END                                                               PAXE 630


      SUBROUTINE PLTXY(X,Y)                                             PLTX  10
C     ***** PLCT COORD. AND CLOSEST EDGE AFTER PROJECTION *****         PLTX  20
      DIMENSION X(3),Y(2)                                               PLTX  30
      REAL*8 CHEM                                                       PLTX  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PLTX  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)PLTX  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PLTX  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PLTX  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PLTX  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PLTX 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     PLTX 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PLTX 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PLTX 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PLTX 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PLTX 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PLTX 160
      T4=1.                                                             PLTX 170
      T1=1.                                                             PLTX 180
      IF(VIEW) 125,125,110                                              PLTX 190
  110 T4=VIEW-X(3)                                                      PLTX 200
      IF(T4) 115,115,120                                                PLTX 210
  115 Y(1)=-99.                                                         PLTX 220
      Y(2)=-99.                                                         PLTX 230
      GO TO 130                                                         PLTX 240
  120 T1=VIEW/T4                                                        PLTX 250
  125 Y(1)=X(1)*T1+XO(1)                                                PLTX 260
      Y(2)=X(2)*T1+XO(2)                                                PLTX 270
      T1=XLNG(1)-ABS(Y(1)*2.-XLNG(1))                                   PLTX 280
      T2=XLNG(2)-ABS(Y(2)*2.-XLNG(2))                                   PLTX 290
      EDGE=AMIN1(T1,T2)*.5                                              PLTX 300
      IF(T4-VIEW*.5) 130,300,300                                        PLTX 310
  130 EDGE=-99.                                                         PLTX 320
  300 RETURN                                                            PLTX 330
      END                                                               PLTX 340


      SUBROUTINE PRELIM                                                 PREL  10
C     ***** DATA INPUT ROUTINE *****                                    PREL  20
      DIMENSION B(9)                                                    PREL  30
      REAL*8 CHEM                                                       PREL  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PREL  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)PREL  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PREL  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PREL  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PREL  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PREL 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     PREL 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PREL 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PREL 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PREL 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PREL 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PREL 160
C     ***** CELL DIMENSIONS *****                                       PREL 170
  106 FORMAT(6F9.6)                                                     PREL 180
      READ (IN,106) (A(I),I=1,6)                                        PREL 190
      T1=ABS(A(4))-1.                                                   PREL 200
      DO 125 J=1,3                                                      PREL 210
      IF(T1) 115,110,110                                                PREL 220
C     ***** CELL ANGLES IN DEGREES *****                                PREL 230
  110 A(J+6)=A(J+3)                                                     PREL 240
      A(J+3)=COS(A(J+6)*1.745329E-2)                                    PREL 250
      GO TO 120                                                         PREL 260
C     ***** COSINES OF CELL ANGLES *****                                PREL 270
  115 A(J+6)=ARCCOS(A(J+3))                                             PREL 280
C     ***** STORE IDEMFACTOR MATRIX *****                               PREL 290
  120 AID(J,J)=1.                                                       PREL 300
      AID(J+1,1)=0.                                                     PREL 310
      AID(J+5,1)=0.                                                     PREL 320
C     ***** STORE METRIC TENSOR *****                                   PREL 330
  125 AA(J,J)=A(J)**2                                                   PREL 340
      AA(1,2)=A(1)*A(2)*A(6)                                            PREL 350
      AA(1,3)=A(1)*A(3)*A(5)                                            PREL 360
      AA(2,3)=A(2)*A(3)*A(4)                                            PREL 370
      AA(2,1)=AA(1,2)                                                   PREL 380
      AA(3,1)=AA(1,3)                                                   PREL 390
      AA(3,2)=AA(2,3)                                                   PREL 400
C     ***** INVERT METRIC TENSOR *****                                  PREL 410
      CALL AXEQB(AA,BB,AID,3)                                           PREL 420
C     ***** CALCULATE RECIPROCAL CELL PARAMETERS *****                  PREL 430
      DO 128 J=1,3                                                      PREL 440
  128 B(J)=SQRT(BB(J,J))                                                PREL 450
      B(6)=BB(1,2)/(B(1)*B(2))                                          PREL 460
      B(5)=BB(1,3)/(B(1)*B(3))                                          PREL 470
      B(4)=BB(2,3)/(B(2)*B(3))                                          PREL 480
      DO 130 J=1,3                                                      PREL 490
  130 B(J+6)=ARCCOS(B(J+3))                                             PREL 500
C     ***** WAS INPUT FOR REAL OR RECIPROCAL CELL *****                 PREL 510
      IF(A(1)-1.) 135,150,150                                           PREL 520
  135 DO 140 J=1,9                                                      PREL 530
      T1=AA(J,1)                                                        PREL 540
      AA(J,1)=BB(J,1)                                                   PREL 550
      BB(J,1)=T1                                                        PREL 560
      T1=A(J)                                                           PREL 570
      A(J)=B(J)                                                         PREL 580
  140 B(J)=T1                                                           PREL 590
C     ***** WRITE OUT CELL PARAMETERS *****                             PREL 600
  143 FORMAT(1H010X,22HDIRECT CELL PARAMETERS/1H 15X,1HA14X,1HB14X,1HC14PREL 610
     1X,5HALPHA10X,4HBETA11X,5HGAMMA)                                   PREL 620
  145 FORMAT(1H 10X,F9.6,2F15.6,3F15.3/1H 48X,6HCOSINEF12.8,2F15.8)     PREL 630
  147 FORMAT(1H010X,26HRECIPROCAL CELL PARAMETERS/1H 15X,2HA*13X,2HB*13XPREL 640
     1,2HC*13X,6HALPHA*9X,5HBETA*10X,6HGAMMA*)                          PREL 650
  150 WRITE (NOUT,143)                                                  PREL 660
      WRITE (NOUT,145) (A(I),I=1,3),(A(I),I=7,9),(A(I),I=4,6)           PREL 670
      WRITE (NOUT,147)                                                  PREL 680
      WRITE (NOUT,145) (B(I),I=1,3),(B(I),I=7,9),(B(I),I=4,6)           PREL 690
C     ***** STORE STANDARD VECTORS *****                                PREL 700
      CALL AXES(AID,AID(1,2),REFV,0)                                    PREL 710
      CALL MM(AA,REFV,AAREV)                                            PREL 720
      DO 160 I=1,3                                                      PREL 730
      DO 160 J=1,3                                                      PREL 740
      AAWRK(J,I)=AAREV(J,I)                                             PREL 750
      Q(J,I)=REFV(I,J)                                                  PREL 760
  160 WRKV(J,I)=REFV(J,I)                                               PREL 770
C     ***** READ AND WRITE SYMMETRY TRANSFORMATIONS *****               PREL 780
  171 FORMAT(1H010X,24HSYMMETRY TRANSFORMATIONS/1H 14X,3HNO.12X,13HTRANSPREL 790
     1FORMED X18X,13HTRANSFORMED Y18X,13HTRANSFORMED Z)                 PREL 800
  173 FORMAT(I1,F14.10,3F3.0,2(F15.10,3F3.0))                           PREL 810
  175 FORMAT(1H 13X,I2,3(F13.6,F4.0,2H XF4.0,2H YF4.0,2H Z))            PREL 820
  177 FORMAT(1H110X,18A4)                                               PREL 830
      WRITE (NOUT,171)                                                  PREL 840
      LINES=14                                                          PREL 850
      DO 190 I=1,48                                                     PREL 860
      LINES=MOD(LINES+1,56)                                             PREL 870
      READ (IN,173) IS,(TS(J,I),(FS(K,J,I),K=1,3),J=1,3)                PREL 880
      IF(LINES) 185,180,185                                             PREL 890
  180 WRITE (NOUT,177) (TITLE(J),J=1,18)                                PREL 900
      WRITE (NOUT,171)                                                  PREL 910
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  185 WRITE (NOUT,175)I,(TS(J,I),(PS(K,J,I),K=1,3),J=1,3)
C     ***** NON-CRYSTALLOGRAPHIC HELIX-SYMMETRY INPUT *****
      IF(PS(3,3,I)-5.)188,186,186
  186 T1=PS(1,3,I)/PS(3,3,I)
      TS(3,I)=TS(3,I)+T1
      T1=AMOD(T1*PS(2,3,I),1.)*6.28318531
      T2=COS(T1)
      T1=SIN(T1)
      DO 187 J=1,9
  187 VT(J,1)=AID(J,1)
      VT(1,1)=T2
      VT(2,2)=T2
      VT(2,1)=-T1
      VT(1,2)=T1
      CALL MM(VT,Q,PAC)
      CALL MM(AAREV,PAC,PS(1,1,I))
  188 IF(IS)195,190,195
  190 CONTINUE
      NG=1
      CALL ERPNT(0.,0)
      I=48
  195 NSYM=I
C     ***** POSITIONAL AND THERMAL PARAMETERS *****
  207 FORMAT(11H0 NO. ATOM 8X,1HX10X,1HY10X,1HZ13X,3HB118X,3HB228X,3HB33
     18X,3HB128X,3HB138X,10HB23    TYPE)
  209 FORMAT(1H I3,1X,A6,3F11.6,5X,6F11.6,F5.0)
  210 FORMAT(1H I3,1X,A6,3F11.6,5X,2F11.6,4F11.0,F5.0)
  211 FORMAT(A6,3X,5F9.6,F9.0)
  213 FORMAT(I1,F8.6,5F9.6,7X,F2.0)
      LINES=LINES+2
      IF(LINES-56)220,215,215
  215 LINES=-1
      GO TO 225
  220 WRITE (NOUT,207)
  225 DO 245 I=1,166
      LINES=MOD(LINES+1,56)
      READ (IN,211)CHEM(I),V1(1),V1(2),(P(J,I),J=1,3),T1
      K=1.+T1
      IF(FLOAT(K-1)-T1)227,228,227
  227 K=1
  228 READ (IN,213)IS,(PA(J,1,I),J=1,7)
      IF(LINES)230,230,232
  230 WRITE (NOUT,177)(TITLE(J),J=1,18)
      WRITE (NOUT,207)
  232 IF(PA(3,1,I)-10000.)235,234,234
  234 WRITE (NOUT,210)I,CHEM(I),(P(J,I),J=1,3),(PA(J,1,I),J=1
     1,7)
      GO TO 238
  235 WRITE (NOUT,209)I,CHEM(I),(P(J,I),J=1,3),(PA(J,1,I),J=1
     1,7)
  238 GO TO (244,239,241,242,244),K
C     ***** TYPE 1 POSITIONAL PARAMETERS (ANGSTROMS) *****
  239 DO 240 J=1,3
  240 P(J,I)=P(J,I)/A(J)
      GO TO 244
C     ***** TYPE 2 POSITIONAL PARAMETERS, STANDARD CARTESIAN *****
  241 V1(1)=P(1,I)
      V1(2)=P(2,I)
      GO TO 243
C     ***** TYPE 3 POSITIONAL PARAMETERS *****
C     ***** CYLINDRICAL COORDINATES REFERRED TO STANDARD CARTESIAN *****
  242 T2=P(2,I)*.01745329252
      V1(1)=V1(1)+P(1,I)*COS(T2)
      V1(2)=V1(2)+P(1,I)*SIN(T2)
  243 V1(3)=P(3,I)
      CALL VM(V1,Q,P(1,I))
  244 IF(IS)246,245,246
  245 CONTINUE
      NG=2
      CALL ERPNT(0.,0)
      I=100
  246 NATOM=I
C     ***** CONVERT TEMP FACTOR COEF TO STANDARD TYPE ZERO *****
      NG1=0
      DO 450 I=1,NATOM
      T1=PA(1,1,I)
      K=1.+PA(7,1,I)
      IF(T1)250,250,255
  250 T1=.1
      GO TO 405
  255 T6=.0506605918
      GO TO(270,260,265,265,270,260,400,405,270,260,270,450),K
C     ***** TYPE 1 *****
  260 DO 262 J=4,6
  262 PA(J,1,I)=PA(J,1,I)*.5
      GO TO 270
C     ***** TYPES 2 AND 3 (BASE 2 SYSTEMS) *****
  265 T6=.351152464
      IF(K-4)270,260,270
C     ***** TYPES 0 THROUGH 5 *****
  270 IF(PA(2,1,I))400,400,272
  272 DO 300 J=1,3
      DO 300 L=J,3
      T2=T6
      IF(K-5)285,275,275
  275 IF(K-6)280,280,281
C     ***** TYPES 4 AND 5 *****
  280 T2=B(J)*B(L)*T2*.25
      GO TO 285
C     ***** TYPES 8 AND 9 (U(I,J) TENSOR SYSTEMS) *****
  281 T2=B(J)*B(L)
      IF(K-11)285,282,282
C     ***** TYPE 10, (CARTESIAN TENSOR SYSTEM) *****
  282 T2=1.0
  285 IF(J-L)290,287,290
  287 VT(J,J)=T2*PA(J,1,I)
      GO TO 300
  290 M=J+L+1
      VT(J,L)=T2*PA(M,1,I)
      VT(L,J)=VT(J,L)
  300 CONTINUE
C     ***** FIND PRINCIPAL AXES *****
      IF(K-11)310,305,305
  305 CALL MM(VT,Q,PAC)
      CALL MM(REFV,PAC,VT)
  310 CALL MM(VT,AA,DA)
      CALL EIGEN(DA,RMS,PAT)
C     ***** ARE EIGENVALUES POSITIVE *****
      IF(RMS(1))325,325,320
  320 IF(NG)350,360,330
  325 NG=3
  330 NG1=1
      CALL ERPNT(FLOAT(I)*100000.+55501.,0)
C     ***** 3 EQUAL EIGENVALUES, USE REFERENCE VECTORS *****
  340 T3=SIGN(SQRT(ABS(RMS(1)+RMS(2)+RMS(3))/3.),RMS(1))
      DO 345 J=1,3
      DO 342 K=1,3
  342 PA(J,K,I)=REFV(J,K)
  345 EV(J,I)=T3
      GO TO 450
  350 IF(NG+6)340,340,352
C     ***** TWO EQUAL EIGENVALUES *****
  352 N=NG+5
      CALL UNIT(PAT(1,N),V1,-1)
      DO 354 K=1,3
      IF(ABS(VMV(V1,AA,REFV(1,K)))-.58)356,354,354
  354 CONTINUE
  356 CALL MM(AA,DA,VT)
      CALL AXES(V1,REFV(1,K),DA,-1)
      DO 359 K=1,3
      L=MOD(N+K-2,3)+1
      DO 358 J=1,3
  358 PA(J,L,I)=DA(J,K)
  359 EV(L,I)=SIGN(SQRT(ABS(VMV(DA(1,K),VT,DA(1,K)))),RMS(L))
      GO TO 450
C     ***** MAKE EIGENVECTORS 1 ANGSTROM LONG *****
  360 CALL AXES(PAT(1,1),PAT(1,3),PA(1,1,I),-1)
  370 NG=0
C     ***** SQRT EIGENVALUE = RMS DISPLACEMENT *****
      DO 375 J=1,3
      T2=RMS(J)
  375 EV(J,I)=SIGN(SQRT(ABS(T2)),T2)
      GO TO 450
C     ***** TYPE 6 (ISOTROPIC TEMP FACTOR) *****
  400 T1=SQRT(T1*1.266515E-2)
C     ***** TYPE 7 (DUMMY SPHERE) *****
  405 DO 410 J=1,3
  410 EV(J,I)=T1
      IF(PA(3,1,I))430,430,415
C     ***** DEFINED VECTORS FOR SPHERE *****
  415 DO 425 J=1,4
      T2=PA(J+2,1,I)
      CALL ATOM(T2,VT(1,J))
      IF(NG)420,425,420
  420 CALL ERPNT(T2,0)
      GO TO 430
  425 CONTINUE
      CALL DIFV(VT(1,2),VT(1,1),V1)
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      CALL DIFV(VT(1,4),VT(1,3),V2)                                     PREL2600
      CALL AXES(V1,V2,PA(1,1,I),-1)                                     PREL2610
      GO TO 450                                                         PREL2620
C     ***** REFERENCE VECTORS FOR SPHERE *****                          PREL2630
  430 DO 435 J=1,9                                                      PREL2640
  435 PA(J,1,I)=REFV(J,1)                                               PREL2650
  450 NG=0                                                              PREL2660
C     ***** WRITE OUT RMS VALUES *****                                  PREL2670
      LINES=LINES+2                                                     PREL2680
      IF(LINES-56)458,458,455                                           PREL2690
  455 LINES=-1                                                          PREL2700
      GO TO 460                                                         PREL2710
  458 WRITE (NOUT,461)                                                  PREL2720
  460 DO 465 I=1,NATOM                                                  PREL2730
      LINES=MOD(LINES+1,56)                                             PREL2740
      IF(LINES)465,462,465                                              PREL2750
  461 FORMAT(10HONO. ATOM 8X,1HX10X,1HY10X,1HZ13X,7HRMSD 1 4X,7HRMSD 2 4PREL2760
     1X,7HRMSD 3 )                                                      PREL2770
  462 WRITE (NOUT,177) (TITLE(J),J=1,18)                                PREL2780
      WRITE (NOUT,461)                                                  PREL2790
  463 FORMAT(1H I3,1X,A6,3F11.6)                                        PREL2800
  465 WRITE (NOUT,209)I,CHEM(I),(P(J,I),J=1,3),(EV(J,I),J=1,3           PREL2810
     1)                                                                 PREL2820
      IF(NG1)999,999,470                                                PREL2830
  470 CALL EXIT                                                         PREL2840
  999 RETURN                                                            PREL2850
      END                                                               PREL2860


      SUBROUTINE PRIME                                                  PRIM  10
C     ****GENERAL INITIALIZATION OF PRIME PARAMETERS****                PRIM  20
      REAL*8 CHEM                                                       PRIM  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PRIM  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)PRIM  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PRIM  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PRIM  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PRIM  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PRIM  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     PRIM 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PRIM 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD PRIM 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PRIM 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PRIM 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PRIM 150
      BRDR=0.5                                                          PRIM 160
C     ****CALCULATE CONSTANTS****                                       PRIM 170
      DO 2999 I=1,5                                                     PRIM 180
 2999 CONT(I)=SQRT(1./(2.*(1.+COS(3.141593   /2.**I))))                 PRIM 190
      DISP=.005                                                         PRIM 200
      FORE=.866                                                         PRIM 210
      IN=5                                                              PRIM 220
      ITILT=0                                                           PRIM 230
      LATM=0                                                            PRIM 240
      NCD=0                                                             PRIM 250
      NG=0                                                              PRIM 260
      NOUT=6                                                            PRIM 270
      NSR=8                                                             PRIM 280
      RES(1)=1.25                                                       PRIM 290
      RES(2)=.5                                                         PRIM 300
      RES(3)=.2                                                         PRIM 310
      SCAL1=1.0                                                         PRIM 320
      SCAL2=1.54                                                        PRIM 330
      SCL=1.54                                                          PRIM 340
      DO 3000 I=1,3                                                     PRIM 350
      SYMB(I,I)=1.                                                      PRIM 360
      SYMB(I+1,1)=0.                                                    PRIM 370
 3000 SYMB(I+5,1)=0.                                                    PRIM 380
      TAPER=.375                                                        PRIM 390
      THETA=0.0                                                         PRIM 400
      VIEW=0.0                                                          PRIM 410
      XLNG(1)=17.0                                                      PRIM 420
      XLNG(2)=11.0                                                      PRIM 430
      XO(1)=8.5                                                         PRIM 440
      XO(2)=5.5                                                         PRIM 450
      DO 3001 J=1,3                                                     PRIM 460
 3001 ORGN(J) = 0.0                                                     PRIM 470
C     ***** INITIATE OVERLAP ROUTINES *****                             PRIM 480
      CALL LAP500(0)                                                    PRIM 490
      RETURN                                                            PRIM 500
      END                                                               PRIM 510


      SUBROUTINE PROJ(D,DP,X,XO,VIEW,I1,I2,I3)                          PROJ  10
C     ***** 3D CARTESIAN TO 2D PLOTTER COORDINATES *****                PROJ  20
      DIMENSION D(3,129),DP(2,129),X(3),XO(3)                           PROJ  30
      T3=VIEW-X(3)                                                      PROJ  40
      DO 145 I=I1,I2,I3                                                 PROJ  50
      T1=D(1,I)+X(1)                                                    PROJ  60
      T2=D(2,I)+X(2)                                                    PROJ  70
      IF(VIEW) 135,135,120                                              PROJ  80
  120 T4=VIEW/(T3-D(3,I))                                               PROJ  90
      T1=T1*T4                                                          PROJ 100
      T2=T2*T4                                                          PROJ 110
  135 DP(1,I)=T1+XO(1)                                                  PROJ 120
  145 DP(2,I)=T2+XO(2)                                                  PROJ 130
      RETURN                                                            PROJ 140
      END                                                               PROJ 150


      SUBROUTINE RADIAL(ND)                                             RADI  10
C     ***** GENERATE ELLIPSE FROM TWO CONJUGATE VECTORS *****           RADI  20
C     ***** ORTHONORMAL VECTORS PRODUCE 8-128 SPOKED CIRCLE *****       RADI  30
C     ***** ND DENOTES NUMBER OF SUBDIVISIONS (1 TO 5) *****            RADI  40
      REAL*8 CHEM                                                       RADI  50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    RADI  60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)RADI  70
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) RADI  80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) RADI  90
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   RADI 100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   RADI 110
      DIMENSION XLNG(3),XO(3),XT(3)                                     RADI 120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   RADI 130
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD RADI 140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1RADI 150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   RADI 160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                RADI 170
      DO 115 J=1,3                                                      RADI 180
      T1=DA(J,1)                                                        RADI 190
      D(J,1)=T1                                                         RADI 200
      D(J,129)=T1                                                       RADI 210
      D(J,65)=-T1                                                       RADI 220
      T1=DA(J,2)                                                        RADI 230
      D(J,33)=T1                                                        RADI 240
  115 D(J,97)=-T1                                                       RADI 250
      DO 135 K=1,ND                                                     RADI 260
      T1=CONT(K)                                                        RADI 270
      KDEL=2**(6-K)                                                     RADI 280
      KDEL1=KDEL+1                                                      RADI 290
      KDEL2=KDEL/2                                                      RADI 300
      DO 135 L=KDEL1,65,KDEL                                            RADI 310
      J=L-KDEL                                                          RADI 320
      M=L-KDEL2                                                         RADI 330
      DO 135 N=1,3                                                      RADI 340
      T2=(D(N,L)+D(N,J))*T1                                             RADI 350
      D(N,M)=T2                                                         RADI 360
  135 D(N,M+64)=-T2                                                     RADI 370
      RETURN                                                            RADI 380
      END                                                               RADI 390


      SUBROUTINE SCRIBE(Y,NPEN,LTNO)                                    SCRI  10
      DIMENSION Y(2),YO(2)                                              SCRI  20
C     ***** SUBROUTINE WHICH LINKS WITH THE PLOTTER-SPECIFIC SUBROUTINESSCRI  30
      IF(NPEN-3) 210,205,205                                            SCRI  40
C     ***** KEEP TRACK OF COORDINATES FOR LAST PEN-UP LOCATION *****    SCRI  50
  205 YO(1)=Y(1)                                                        SCRI  60
      YO(2)=Y(2)                                                        SCRI  70
      NPO=0                                                             SCRI  80
      RETURN                                                            SCRI  90
  210 IF(LTNO) 230,245,215                                              SCRI 100
C     ***** CALL MECHANICAL PLOTTER PLOTTING SUBROUTINE *****           SCRI 110
  215 IF(NPO) 225,220,225                                               SCRI 120
  220 CALL PLOT(YO(1),YO(2),3)                                          SCRI 130
  225 CALL PLOT(Y(1),Y(2),2)                                            SCRI 140
      GO TO 245                                                         SCRI 150
C     ***** CALL CRT PLOTTING SUBROUTINE *****                          SCRI 160
  230 IF(NPO) 240,235,240                                               SCRI 170
  235 CALL CRT(YO(1),YO(2),0,1)                                         SCRI 180
  240 CALL CRT(Y(1),Y(2),-LTNO,1)                                       SCRI 190
  245 NPO=1                                                             SCRI 200
      RETURN                                                            SCRI 210
      END                                                               SCRI 220


      SUBROUTINE SEARC                                                  SEAR  10
      DIMENSION NW(6),DX(3),S(2,200),U(3),V(3),W(2,4),WW(2,3),X(4),Y(3) SEAR  20
      DIMENSION Z(3)                                                    SEAR  30
      REAL*8 CHEM                                                       SEAR  40
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      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
      DIMENSION XLNG(3),XO(3),XT(3)
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
C     ***** OBTAIN PROBLEM PARAMETERS *****
      WRITE (NOUT,20)
   20 FORMAT(1H0 9X,82H          FROM ATOMS    TO ATOMS     WITH RADIUS OR
     1, IF A BOX, WITH SEMIDIMENSIONS  /11X,46HCODE   (MIN  MAX)   (MIN
     2 MAX)                  7X,1HA8X,1HB8X,1HC)
      IF(AIN(1)-10000.)100,100,101
  100 ITOM1=AIN(1)
      SYITOM=55501.
      GO TO 103
  101 ITOM1=AIN(1)/100000.
      SYITOM=AMOD(AIN(1),100000.)
  102 IF(ABS(AIN(2))-10000.) 103,103,104
  103 ITOM2 = ABS(AIN(2))
      SYITO2=SYITOM
      GO TO 105
  104 ITOM2=ABS(AIN(2))/100000.
      SYITO2=AMOD(ABS(AIN(2)),100000.)
  105 ITAR1=AIN(3)
      IF(ITAR1) 108,108,110
  108 ITAR1=1
  110 ITAR2=AIN(4)
      DMAX=AIN(5)
      IF(DMAX) 115,115,120
  115 DMAX=4.
      AIN(5)=DMAX
  120 DMX=DMAX*DMAX
      TEM=.01
      KFUN=NJ*100+MOD(NJ2,10)
      K=NJ*100+NJ2
      I0=SYITOM
      I02=SYITO2
      LATOM=LATM
  121 FORMAT(1H010X,2I3,I5,I4,I5,2I4,18X,3F9.3/1H )
      WRITE (NOUT,121)K,ITOM1,I0,ITOM2,I02,
     1ITAR1,ITAR2,(AIN(J),J=5,7)
  124 FORMAT(1H 15X,2I5,I8,I5,2F9.3)
      IF(NCD) 130,130,125
  125 WRITE (NOUT,124) ((KD(J,I),J=1,4),(CD(J,I),J=1,2) ,I=1,
     1NCD)
  130 DO 135 J=1,4
      W(1,J)=99.
  135 W(2,J)=-99.
      DO 155 I=ITAR1,ITAR2
      T1=FLOAT(I)*100000.
      CALL ATOM(T1,X)
      IF(NG) 140,145,140
  140 CALL ERPNT(T1,KFUN)
      GO TO 600
  145 X(4)=X(1)-X(2)
      DO 155 J=1,4
      TEM=X(J)
      IF(W(2,J)-TEM) 148,150,150
  148 W(2,J)=TEM
  150 IF(TEM-W(1,J)) 152,155,155
  152 W(1,J)=TEM
  155 CONTINUE
      KFUN2=MOD(KFUN,10)
      GO TO (165,165,160,156,165,165),KFUN2
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES TRICLINIC BOX *****
  156 DO 158 J=1,3
  158 DX(J)=AIN(J+4)
      GO TO 170
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES RECTANGULAR BOX *****
  160 DO 162 J=1,3
      DX(J)=0.
      DO 162 I=1,3
  162 DX(J)=DX(J)+ABS(REFV(J,I)*AIN(I+4))
      GO TO 170
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES DMAX SPHERE *****
  165 T1=1.-A(4)*A(4)-A(5)*A(5)-A(6)*A(6)+2.*A(4)*A(5)*A(6)
      DO 168 J=1,3
  168 DX(J)=SQRT((1.-A(J+3)**2)/T1)*DMAX/A(J)
C     ***** START SEARCH AROUND REFERENCE ATOMS *****
  170 LIST=0
      LAST=0
      M1=ITOM1
      N1=ITOM2
      IF(KFUN2-5) 186,172,172
C     ***** CONVOLUTE AND REITERATIVE CONVOLUTE INSTRUCTIONS *****
  172 IF(LATM) 174,174,176
C     ***** FAULT, NO ENTRIES IN ATOMS LIST *****
  174 NG=12
      CALL ERPNT(0.,KFUN)
      GO TO 600
C     ***** CHECK FOR REFERENCE ATOMS IN ATOMS LIST *****
  176 IF(LATM-LAST)600,600,177
  177 LIST=LAST
      LAST=LATM
  178 LIST=LIST+1
      IF(LAST-LIST) 505,180,180
  180 T1=ATOMS(1,LIST)
      ITOM=T1/100000.
      IF(ITOM-ITOM1) 178,184,182
  182 IF(ITOM2-ITOM) 178,184,184
  184 SYITOM=AMOD(T1,100000.)
      SYITO2=SYITOM
      M1=ITOM
      N1=ITOM
C     ***** SET INITIAL RUN PARAMETERS *****
  186 M2=AMOD(SYITOM,100.)
      M5=AMOD(SYITOM/100.,1000.)
      M3=M5/100
      M4=MOD(M5/10,10)
      M5=MOD(M5,10)
C     ***** SET TERMINAL RUN PARAMETERS *****
      N2=AMOD(SYITO2,100.)
      N5=AMOD(SYITO2/100.,1000.)
      N3=N5/100
      N4=MOD(N5/10,10)
      N5=MOD(N5,10)
C     ***** START SEARCH AROUND REFERENCE ATOMS *****
      DO 500 L5=M5,N5
      DO 500 L4=M4,N4
      DO 500 L3=M3,N3
      DO 500 L2=M2,N2
      DO 500 ITOM=M1,N1
      T1=FLOAT(ITOM)*100000.+FLOAT(L3*10000+L4*1000+L5*100+L2)
      CALL ATOM(T1,Y)
      IF(NG) 188,190,188
  188 CALL ERPNT(T1,KFUN)
      GO TO 500
C     ***** K=SYMMETRY EQUIVALENT POSITION *****
  190 NUM=0
      DO 400 K=1,NSYM
C     ***** SUBTRACT SYMMETRY TRANSLATION FROM REFERENCE ATOM *****
      DO 192 J=1,3
  192 U(J)=Y(J)-TS(J,K)
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****
      DO 200 J=1,3
      DO 200 L=1,2
      WW(L,J)=0.0
      DO 200 I=1,3
      TEM=FS(I,J,K)
      IF(TEM) 194,200,196
  194 N=MOD(L,2)+1
      GO TO 198
  196 N=L
  198 WW(L,J)=WW(L,J)+W(N,I)*TEM
  200 CONTINUE
C     ***** CHECK FOR MIXED INDEX TRANSFORMATION *****
      DO 215 J=1,2
      TEM=FS(1,J,K)
      IF(TEM+FS(2,J,K)) 215,201,215
  201 IF(TEM) 203,215,207
  203 WW(1,J)=W(2,4)*TEM
      WW(2,J)=W(1,4)*TEM
      GO TO 215
  207 WW(1,J)=W(1,4)*TEM
      WW(2,J)=W(2,4)*TEM
  215 CONTINUE
C     ***** MOVE 4 CELLS AWAY THEN MOVE BACK UNTIL PARALLELEPIPED AROUND
C         REF ATOM AND BOX AROUND TRANSFORMED ASYM UNIT INTERSECT *****
      N=0
      DO 235 J=1,3
      DO 225 I=1,2
      N=N+1
      TT=(U(J)-WW(I,J))*FLOAT(I*2-3)-DX(J)
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      TEM=5.0                                                           SEAR1750
  221 TEM=TEM-1.0                                                       SEAR1760
      IF(TEM+TT) 225,225,221                                            SEAR1770
  225 NW(N)=TEM*FLOAT(I*2-3)+5.                                         SEAR1780
C     ***** IF NO POSSIBILITY OF A HIT, GO TO NEXT SYMMETRY OPER *****  SEAR1790
      IF(NW(N)-NW(N-1))400,235,235                                      SEAR1800
  235 CONTINUE                                                          SEAR1810
      LL=NW(1)                                                          SEAR1820
      LU=NW(2)                                                          SEAR1830
      ML=NW(3)                                                          SEAR1840
      MU=NW(4)                                                          SEAR1850
      NL=NW(5)                                                          SEAR1860
      NU=NW(6)                                                          SEAR1870
C     ***** L CELL TRANSLATIONS IN X *****                              SEAR1880
      DO 395 L=LL,LU                                                    SEAR1890
      V(1)=U(1)+FLOAT(L-5)                                              SEAR1900
C     ***** M CELL TRANSLATIONS IN Y *****                              SEAR1910
      DO 395 M=ML,MU                                                    SEAR1920
      V(2)=U(2)+FLOAT(M-5)                                              SEAR1930
C     ***** N CELL TRANSLATIONS IN Z *****                              SEAR1940
      DO 395 NN=NL,NU                                                   SEAR1950
      V(3)=U(3)+FLOAT(NN-5)                                             SEAR1960
C     ***** I = TARGET ATOM *****                                       SEAR1970
      DO 395 I=ITAR1,ITAR2                                              SEAR1980
      DO 250 J=1,3                                                      SEAR1990
      TEM=0.0                                                           SEAR2000
      DO 245 II=1,3                                                     SEAR2010
  245 TEM=TEM+PS(II,J,K)*P(II,I)                                        SEAR2020
C     ***** SEE IF WITHIN PARALLELEPIPED*****                           SEAR2030
      TEM=TEM-V(J)                                                      SEAR2040
      IF(DX(J)-ABS(TEM))395,250,250                                     SEAR2050
  250 X(J)=TEM                                                          SEAR2060
      GO TO (255,255,252,277,255,255),KFUN2                             SEAR2070
C     ***** SEE IF WITHIN MODEL BOX *****                               SEAR2080
  252 CALL VM(X,AAREV,V1(2))                                            SEAR2090
      DO 253 J=2,4                                                      SEAR2100
      IF(AIN(J+3)-ABS(V1(J)))395,253,253                                SEAR2110
  253 CONTINUE                                                          SEAR2120
      GO TO 277                                                         SEAR2130
C     ***** SEE IF WITHIN SPHERE *****                                  SEAR2140
  255 DSQ=VMV(X,AA,X)                                                   SEAR2150
      IF(DMX-DSQ)395,256,256                                            SEAR2160
  256 IF(DSQ-.0001)258,260,260                                          SEAR2170
  258 IF(KFUN-402)395,260,260                                           SEAR2180
  260 TEM=SQRT(DSQ)                                                     SEAR2190
      IF(AIN(8))265,265,261                                             SEAR2200
C     *****SELECT ONLY FIRST ASYMMETRIC UNIT ENCOUNTERED *****          SEAR2210
  261 IF(LATM)265,265,262                                               SEAR2220
  262 ZMIN=FLOAT(I)*100000.                                             SEAR2230
      ZMAX=ZMIN+100000.                                                 SEAR2240
      DO 264 J=1,LATM                                                   SEAR2250
      ZSTO=ATOMS(1,J)                                                   SEAR2260
      IF(ZSTO-ZMIN)264,263,263                                          SEAR2270
  263 IF(ZMAX-ZSTO)264,264,395                                          SEAR2280
  264 CONTINUE                                                          SEAR2290
C     ***** SELECT VECTORS ACCORDING TO CODES IF ANY *****              SEAR2300
  265 IF(NCD)277,277,268                                                SEAR2310
  268 DO 275 J=1,NCD                                                    SEAR2320
  269 IF(ITOM-KD(1,J))275,270,270                                       SEAR2330
  270 IF(KD(2,J)-ITOM)275,271,271                                       SEAR2340
  271 IF(I-KD(3,J))    275,272,272                                      SEAR2350
  272 IF(KD(4,J)-I)    275,273,273                                      SEAR2360
  273 IF(TEM-CD(1,J))  275,274,274                                      SEAR2370
  274 IF(CD(2,J)-TEM)  275,277,277                                      SEAR2380
  275 CONTINUE                                                          SEAR2390
      GO TO 395                                                         SEAR2400
  277 V1(1) = 100000.*FLOAT(I)+FLOAT((1110-L*100-M*10-NN)*100+K)        SEAR2410
      IF(KFUN-402)278,325,325                                           SEAR2420
C     ***** DETERMINE CORRECT POSITION IN SORTED VECTOR TABLE *****     SEAR2430
  278 IF(NUM)317,317,279                                                SEAR2440
  279 DO 315 II=1,NUM                                                   SEAR2450
      TT=S(2,II)-TEM                                                    SEAR2460
      IF(ABS(TT)-0.0001)297,297,281                                     SEAR2470
  281 IF(TT)315,297,283                                                 SEAR2480
C     ***** MOVE LONGER VECTORS TOWARD END OF TABLE *****               SEAR2490
  283 IF(200-NUM)287,287,289                                            SEAR2500
  287 NUM=199                                                           SEAR2510
  289 IJ=NUM                                                            SEAR2520
      DO 295 J=II,NUM                                                   SEAR2530
      S(1,IJ+1)=S(1,IJ)                                                 SEAR2540
      S(2,IJ+1)=S(2,IJ)                                                 SEAR2550
  295 IJ=IJ-1                                                           SEAR2560
      GO TO 319                                                         SEAR2570
C     ***** CHECK FOR DUPLICATE VECTORS IF DISTANCES ARE EQUAL *****    SEAR2580
  297 CALL ATOM(S(1,II),Z)                                              SEAR2590
      DO 305 J=1,3                                                      SEAR2600
      IF(ABS(X(J)+Y(J)-Z(J))-0.0001)305,305,315                         SEAR2610
  305 CONTINUE                                                          SEAR2620
      GO TO 395                                                         SEAR2630
  315 CONTINUE                                                          SEAR2640
      IF(200-NUM)320,320,317                                            SEAR2650
C     ***** STORE THE RESULT IN VECTOR TABLE *****                      SEAR2660
  317 II=NUM+1                                                          SEAR2670
  319 NUM=NUM+1                                                         SEAR2680
      S(1,II)=V1(1)                                                     SEAR2690
      S(2,II)=TEM                                                       SEAR2700
  320 IF(KFUN-106)395,325,325                                           SEAR2710
C     ***** STORE RESULT IN ATOMS TABLE *****                           SEAR2720
  325 DO 330 J=1,3                                                      SEAR2730
  330 V1(J+1)=X(J)+Y(J)                                                 SEAR2740
      CALL STOR                                                         SEAR2750
  395 CONTINUE                                                          SEAR2760
  400 CONTINUE                                                          SEAR2770
C     ***** PRINT OUT DISTANCES *****                                   SEAR2780
  421 FORMAT(1H010X,20HVECTORS FROM ATOM  (I3,1H,I5,1H)6X,8HTO ATOMSI4, SEAR2790
     18H THROUGHI4)                                                     SEAR2800
      IO = AMOD(T1,100000.)                                             SEAR2810
      WRITE (NOUT,421)ITOM,IO,ITAR1,ITAR2                               SEAR2820
      IF(NUM)500,500,423                                                SEAR2830
  423 DO 435 I=1,NUM                                                    SEAR2840
      T2=S(1,I)                                                         SEAR2850
      I1=T2/100000.                                                     SEAR2860
      I2=T2-FLOAT(I1)*100000.                                           SEAR2870
      CALL ATOM(T2,Z)                                                   SEAR2880
      IF(I-1)432,432,434                                                SEAR2890
  427 FORMAT(1H 13X,2(A6,1X),39X,1H(I3,1H,I5,1H)3F7.4,7X,3HD =F6.3)     SEAR2900
  429 FORMAT(1H 13X,2(A6,1X),2(3H  (I3,1H,I5,1H)3F7.4,3X),4X,3HD =F6.3) SEAR2910
  432 WRITE (NOUT,429)CHEM(ITOM),CHEM(I1),ITOM,IO,(Y(J),J=1,3           SEAR2920
     1),I1,I2,(Z(J),J=1,3),S(2,I)                                       SEAR2930
      GO TO 435                                                         SEAR2940
  434 WRITE (NOUT,427)CHEM(ITOM),CHEM(I1),I1,I2,(Z(J),J=1,3),           SEAR2950
     1S(2,I)                                                            SEAR2960
  435 CONTINUE                                                          SEAR2970
C     ***** CALCULATE ANGLES ABOUT REF ATOM IF CODE IS 102 *****        SEAR2980
  437 IF(KFUN-102)500,451,500                                           SEAR2990
  441 FORMAT(1H010X,18HANGLES ARCUND ATOMI5)                            SEAR3000
  451 WRITE (NOUT,441)ITOM                                              SEAR3010
      L=NUM-1                                                           SEAR3020
      IF(L)500,500,457                                                  SEAR3030
  457 DO 465 I=1,L                                                      SEAR3040
      T2=S(1,I)                                                         SEAR3050
      T3=S(2,I)                                                         SEAR3060
      I1=T2/100000.                                                     SEAR3070
      I2=T2-FLOAT(I1)*100000.                                           SEAR3080
      CALL ATOM(T2,X)                                                   SEAR3090
      CALL DIFV(X,Y,U)                                                  SEAR3100
      CALL MV(AA,U,V2)                                                  SEAR3110
      M=I+1                                                             SEAR3120
      DO 465 J=M,NUM                                                    SEAR3130
      T4=S(1,J)                                                         SEAR3140
      J1=T4/100000.                                                     SEAR3150
      J2=T4-FLOAT(J1)*100000.                                           SEAR3160
      CALL ATOM(T4,Z)                                                   SEAR3170
      CALL DIFV(Z,Y,V)                                                  SEAR3180
      F=ARCCOS(VV(V,V2)/(T3*S(2,J)))                                    SEAR3190
      CALL DIFV(X,Z,V3)                                                 SEAR3200
      F1=SQRT(VMV(V3,AA,V3))                                            SEAR3210
  460 FORMAT(1H 13X,3(A6,1X),7X,3(2H (I3,1H,I5,1H)),12X,3HD =F6.3,7X,3HASEAR3220
     1 =F6.2)                                                           SEAR3230
  465 WRITE (NOUT,460)CHEM(I1),CHEM(ITOM),CHEM(J1),I1,I2,ITOM           SEAR3240
     1,IO,J1,J2,F1,F                                                    SEAR3250
  495 CONTINUE                                                          SEAR3260
  500 CONTINUE                                                          SEAR3270
      IF(LAST-LIST)505,505,178                                          SEAR3280
  505 IF(KFUN2-6)600,176,600                                            SEAR3290
  600 IF(KFUN-106)610,605,610                                           SEAR3300
  605 LATM=LATOM                                                        SEAR3310
  610 RETURN                                                            SEAR3320
      END                                                               SEAR3330


      SUBROUTINE SPARE(INST)                                            SPAR  10
C     ***** INSTRUCTION 1201 PRODUCES PUNCHED CARDS WITH POSIT.+THERMAL SPAR  20
C     ***** PARAMETERS FOR ATOMS PLACED IN THE ATOMS LIST BY THE 400    SPAR  30
C     ***** SERIES INSTRUCTIONS                                         SPAR  40
      REAL*8 CHEM                                                       SPAR  50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    SPAR  60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)SPAR  70
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      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) SPAR  80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) SPAR  90
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   SPAR 100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   SPAR 110
      DIMENSION XLNG(3),XO(3),XT(3)                                     SPAR 120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   SPAR 130
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD SPAR 140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1SPAR 150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   SPAR 160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                SPAR 170
      REAL*8 CHM                                                        SPAR 180
C     ***** FIRST FIELD ON INSTRUCTION CARD = NO. OF POSITION PARAMETER SPAR 190
C     ***** CARDS TO BE READ BY THIS SUBROUTINE (STANDARD CRPLS FORMAT) SPAR 200
C     ***** THE SEQUENCE OF THESE CARDS NEED NOT BE IDENTICAL WITH      SPAR 210
C     ***** THE ORIGINAL INPUT ATOM DECK SEQUENCE                       SPAR 220
      IF(INST-1201) 100,105,100                                         SPAR 230
  100 NG = 9                                                            SPAR 240
      RETURN                                                            SPAR 250
  105 IF(AIN(1)) 100,100,115                                            SPAR 260
  115 LAST = AIN(1)                                                     SPAR 270
      DO 150 L=1,LAST                                                   SPAR 280
      READ (IN,116) CHM,V2(1),V2(2),(V1(J),J=1,4)                       SPAR 290
  116 FORMAT(A6,3X,6F9.6)                                               SPAR 300
      WRITE (NOUT,117) CHM,V2(1),V2(2),(V1(J),J=1,4)                    SPAR 310
  117 FORMAT(1H0,24X,25HOLD POSITION PARAMETERS  ,A6,4X,6F10.6)         SPAR 320
C     ***** FIND ATOM NUMBER *****                                      SPAR 330
      DO 125 IA=1,NATOM                                                 SPAR 340
      DO 120 J=1,3                                                      SPAR 350
      IF(ABS(V1(J)-P(J,IA))-0.001) 120,120,125                          SPAR 360
  120 CONTINUE                                                          SPAR 370
      IX = IA                                                           SPAR 380
      GO TO 130                                                         SPAR 390
  125 CONTINUE                                                          SPAR 400
      GO TO 150                                                         SPAR 410
C     ***** SEARCH ATOMS LIST FOR ENTRIES WITH ATOM NUMBER IX *****     SPAR 420
  130 IF(LATM) 150,150,131                                              SPAR 430
  131 DO 145 IB=1,LATM                                                  SPAR 440
      T1 = ATOMS(1,IB)                                                  SPAR.450
      IF(IX-INT(T1/100000.)) 145,135,145                                SPAR 460
  135 CALL ATOM(T1,V1)                                                  SPAR 470
      WRITE (NOUT,136) T1,CHM,V2(1),V2(2),(V1(J),J=1,4)                 SPAR 480
  136 FORMAT(1H0,9X,F10.0,5X,25HNEW POSITION PARAMETERS  ,A6,4X,6F10.6) SPAR 490
      I1 = T1                                                           SPAR 500
      PUNCH 137, CHM,V2(1),V2(2),(V1(J),J=1,4),I1                       SPAR 510
  137 FORMAT(A6,3X,6F9.6,9X,I8)                                         SPAR 520
      CALL PAXES(T1,-1)                                                 SPAR 530
      DO 140 I=1,3                                                      SPAR 540
      DO 140 J=1,3                                                      SPAR 550
  140 Q(J,I) = Q(J,I) /.0506605918                                      SPAR 560
      WRITE (NOUT,141) Q(1,1),Q(2,2),Q(3,3),Q(1,2),Q(1,3),Q(2,3)        SPAR 570
  141 FORMAT(1H ,24X,25HNEW THERMAL PARAMETERS   ,6F10.6)               SPAR 580
      PUNCH 142, Q(1,1),Q(2,2),Q(3,3),Q(1,2),Q(1,3),Q(2,3),I1           SPAR 590
  142 FORMAT(6F9.6,18X,I8)                                              SPAR 600
  145 CONTINUE                                                          SPAR 610
  150 CONTINUE                                                          SPAR 620
  300 RETURN                                                            SPAR 630
      END                                                               SPAR 640


      SUBROUTINE STOR                                                   STOR  10
C     ***** STORE IN OR REMOVE FROM ATOMS ARRAY *****                   STOR  20
      REAL*8 CHM                                                        STOR  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    STOR  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)STOR  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) STOR  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) STOR  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   STOR  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   STOR  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     STOR 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   STOR 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD STOR 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1STOR 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   STOR 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                STOR 150
      IF(LATM) 481,481,450                                              STOR 160
  450 IF(500-LATM) 455,455,460                                          STOR 170
  455 IF(NJ2-10) 490,490,460                                            STOR 180
  460 L=LATM                                                            STOR 190
C     ***** CHECK FOR POSITIONAL DUPLICATION *****                      STOR 200
      DO 480 K=1,L                                                      STOR 210
      DO 465 J=2,4                                                      STOR 220
      IF(ABS(V1(J)-ATOMS(J,K))-0.001) 465,465,480                       STOR 230
  465 CONTINUE                                                          STOR 240
      IF(NJ2-10) 490,490,470                                            STOR 250
C     ***** ATOM REMOVAL BY TABLE PUSHDOWN *****                        STOR 260
  470 LATM=LATM-1                                                       STOR 270
      DO 475 I=K,LATM                                                   STOR 280
      DO 475 J=1,4                                                      STOR 290
  475 ATOMS(J,I)=ATOMS(J,I+1)                                           STOR 300
      GO TO 490                                                         STOR 310
  480 CONTINUE                                                          STOR 320
  481 IF(NJ2-10) 482,490,490                                            STOR 330
C     ***** STORE ATOM *****                                            STOR 340
  482 IF(499-LATM) 490,483,485                                          STOR 350
  483 NG=16                                                             STOR 360
      CALL ERPNT (V1(1),400)                                            STOR 370
  485 LATM=LATM+1                                                       STOR 380
      DO 486 J=1,4                                                      STOR 390
  486 ATOMS(J,LATM)=V1(J)                                               STOR 400
  490 RETURN                                                            STOR 410
      END                                                               STOR 420


      SUBROUTINE TMM(X,Y,Z)                                             TMM   10
C     ***** TRANSPOSE(TRANSPOSE(X)*Y)=Z *****                           TMM   20
C     ***** X,Y,Z ARE 3X3 MATRICES *****                                TMM   30
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                    TMM   40
      DO 115 I=1,3                                                      TMM   50
      DO 115 K=1,3                                                      TMM   60
  115 Z(K,I)=X(1,I)*Y(1,K)+X(2,I)*Y(2,K)+X(3,I)*Y(3,K)                  TMM   70
      RETURN                                                            TMM   80
      END                                                               TMM   90


      SUBROUTINE UNIT(X,Z,ITYPE)                                        UNIT  10
      DIMENSION X(3),Y(3),Z(3)                                          UNIT  20
      REAL*8 CHEM                                                       UNIT  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    UNIT  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)UNIT  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) UNIT  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) UNIT  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   UNIT  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   UNIT  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     UNIT 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   UNIT 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD UNIT 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1UNIT 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   UNIT 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                UNIT 150
      Y(1)=X(1)                                                         UNIT 160
      Y(2)=X(2)                                                         UNIT 170
      Y(3)=X(3)                                                         UNIT 180
      IF(ITYPE) 125,125,105                                             UNIT 190
  105 T1=SQRT(Y(1)*Y(1)+Y(2)*Y(2)+Y(3)*Y(3))                            UNIT 200
      GO TO 145                                                         UNIT 210
  125 T1=SQRT(Y(1)*(Y(1)*AA(1,1)+Y(2)*(AA(1,2)+AA(2,1))+Y(3)*(AA(1,3)+A UNIT 220
     1A(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2)))+Y(3)*Y(3)*AA(3UNIT 230
     2,3))                                                              UNIT 240
  145 IF(T1) 155,155,175                                                UNIT 250
  155 NG=5                                                              UNIT 260
      GO TO 300                                                         UNIT 270
  175 Z(1)=Y(1)/T1                                                      UNIT 280
      Z(2)=Y(2)/T1                                                      UNIT 290
      Z(3)=Y(3)/T1                                                      UNIT 300
  300 RETURN                                                            UNIT 310
      END                                                               UNIT 320


      SUBROUTINE VM(X,Y,Z)                                              VM    10
C     TRANSPOSED VECTOR TIMES MATRIX                                    VM    20
C     Z(3)=X(3)*Y(3,3)                                                  VM    30
      DIMENSION X(3),Y(3,3),Z(3)                                        VM    40
      DO 115 J=1,3                                                      VM    50
      Z(J)=0.0                                                          VM    60
      DO 115 I=1,3                                                      VM    70
  115 Z(J)=Z(J)+X(I)*Y(I,J)                                             VM    80
      RETURN                                                            VM    90
      END                                                               VM   100


      FUNCTION VMV(X1,Q,X2)                                             VMV   10
C     TRANSPOSED VECTOR * MATRIX * VECTOR                               VMV   20
C     VMV=X1(3)*Q(3,3)*X2(3)     TO  EVALUATE QUADRATIC OR BILINEAR FORM VMV   30
      DIMENSION X1(3),Q(3,3),X2(3)                                      VMV   40
      T1=0.                                                             VMV   50
      DO 10 J=1,3                                                       VMV   60
   10 T1=T1+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))              VMV   70
      VMV=T1                                                            VMV   80
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      RETURN                                                            VMV   90
      END                                                               VMV  100


      FUNCTION VV(X,Y)                                                  VV    10
C     TRANSPOSED VECTOR * VECTOR                                        VV    20
C     VV=X(3)*Y(3)                                                      VV    30
      DIMENSION X(3),Y(3)                                               VV    40
      VV=X(1)*Y(1)+X(2)*Y(2)+X(3)*Y(3)                                  VV    50
      RETURN                                                            VV    60
      END                                                               VV    70


      SUBROUTINE XYZ(QA,X,ITYPE)                                        XYZ   10
C     ***** ITYPE .GT.0 CART. COORD. FROM ATOM CODE WORD *****          XYZ   20
C     ***** XABSF(ITYPE) .LE.2 FOR WORKING SYSTEM *****                 XYZ   30
C     ***** XABSF(ITYPE) .GT.2 FOR REFERENCE SYSTEM *****               XYZ   40
C     ***** ITYPE .LE.0 USES TRICLINIC COORD. XT *****                  XYZ   50
      DIMENSION X(3)                                                    XYZ   60
      REAL*8 CHEM                                                       XYZ   70
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    XYZ   80
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)XYZ   90
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) XYZ  100
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) XYZ  110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   XYZ  120
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   XYZ  130
      DIMENSION XLNG(3),XO(3),XT(3)                                     XYZ  140
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   XYZ  150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD XYZ  160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1XYZ  170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   XYZ  180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                XYZ  190
      IT=IABS(ITYPE)-2                                                  XYZ  200
      NG1=NG                                                            XYZ  210
      NG=0                                                              XYZ  220
      IF(ITYPE)10,10,5                                                  XYZ  230
    5 CALL ATOM(QA,XT)                                                  XYZ  240
      IF(NG)30,10,30                                                    XYZ  250
   10 T1=0.                                                             XYZ  260
      DO 15 J=1,3                                                       XYZ  270
      T2=XT(J)-ORGN(J)                                                  XYZ  280
      V1(J)=T2                                                          XYZ  290
   15 T1=T1+ABS(T2)                                                     XYZ  300
      IF(T1-.0001)20,20,40                                              XYZ  310
   20 NG=NG1                                                            XYZ  320
   30 DO 35 J=1,3                                                       XYZ  330
   35 X(J)=0.                                                           XYZ  340
      GO TO 300                                                         XYZ  350
   40 IF(IT)45,45,60                                                    XYZ  360
C     ***** RELATIVE TO WORKING SYSTEM *****                            XYZ  370
   45 DO 55 I=1,3                                                       XYZ  380
      T1=0.                                                             XYZ  390
      DO 50 J=1,3                                                       XYZ  400
   50 T1=T1+V1(J)*AAWRK(J,I)                                            XYZ  410
   55 X(I)=T1*SCAL1                                                     XYZ  420
      GO TO 300                                                         XYZ  430
C     ***** RELATIVE TO REFERENCE SYSTEM *****                          XYZ  440
   60 DO 70 I=1,3                                                       XYZ  450
      T1=0.                                                             XYZ  460
      DO 65 J=1,3                                                       XYZ  470
   65 T1=T1+V1(J)*AAREV(J,I)                                            XYZ  480
   70 X(I)=T1*SCAL1                                                     XYZ  490
  300 RETURN                                                            XYZ  500
      END                                                               XYZ  510


      SUBROUTINE CRT(X1,Y1,I1,I2)                                       CRT   10
C     ***** DUMMY SUBROUTINE TO REPLACE THE CATHODE-RAY-TUBE PACKAGE ***CRT   20
C     ***** SUBROUTINE CRT IS CALLED BY SUBROUTINES F200 AND DRAW ***** CRT   30
      RETURN                                                            CRT   40
      END                                                               CRT   50


      SUBROUTINE IDAY(H2)                                               IDAY  10
C     ***** DUMMY FOR ORNL LOCAL SUBROUTINE CALLED BY F200 FOR CRT IDENTIDAY  20
C     ***** IDAY OBTAINS DATE (8 BCD CHARACTERS) FROM OPERATING SYSTEM  IDAY  30
      RETURN                                                            IDAY  40
      END                                                               IDAY  50
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      SUBROUTINE JOBNUM(H1)                                             JOBN  10
C     ***** DUMMY FOR ORNL LOCAL SUBROUTINE CALLED BY F200 FOR CRT IDENTJOBN  20
C     ***** JOBNUM OBTAINS USERS JOB NUMBER (4 BCD CHARACTERS) *****    JOBN  30
      RETURN                                                            JOBN  40
      END                                                               JOBN  50


 CUBANE  E.B.FLEISCHER   1964  J.A.C.S.  86,3889                        EXAM  10
    5.34      5.34      5.34     72.26     72.26     72.26              EXAM  20
          0  1  0  0               0  0  1  0               0  0  0  1EXAM  30
          0  0  0  1               0  1  0  0               0  0  1  0EXAM  40
          0  0  1  0               0  0  0  1               0  1  0  0EXAM  50
          0 -1  0  0               0  0 -1  0               0  0  0 -1EXAM  60
          0  0  0 -1               0 -1  0  0               0  0 -1  0EXAM  70
1         0  0 -1  0               0  0  0 -1               0 -1  0  0EXAM  80
  C1                              -.18711   .19519   .10706 0           EXAM  90
  .04100   .04250   .04500  -.00420  -.01420  -.00510       0           EXAM 100
  C2                               .11546   .11546   .11546 0           EXAM 110
  .04680   .04680   .04680  -.01430  -.01430  -.01430       0           EXAM 120
  H1                              -.32460   .34680   .18480 0           EXAM 130
     .10                                                    7           EXAM 140
  H2                               .21000   .21000   .21000 0           EXAM 150
     .10                                                    7           EXAM 160
 ORGN                                   0         0         0 0         EXAM 170
1                                                           0           EXAM 180
  3   101  155501         2         1         4       3.61              EXAM 190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****      EXAM 200
  3   102  155501         2         1         4       1.8               EXAM 210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****          EXAM 220
  3   201                                                               EXAM 230
***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****  EXAM 240
  3   301       11.       11.       30.       1.5                       EXAM 250
***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****  EXAM 260
  3   303                                                               EXAM 270
***** ELIMINATE ALL RETRACING *****                                     EXAM 280
  3   402  555501         5         1         4       3.2               EXAM 290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****   EXAM 300
  3   501  555501   255501   155501   255501   155502                  0EXAM 310
***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****EXAM 320
  3   502         2       25.         1       28.                       EXAM 330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****      EXAM 340
  3   604         0         0         0     1.54                        EXAM 350
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **EXAM 360
  3   503         2       2.7                                           EXAM 370
***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****         EXAM 380
  3  1101                                                               EXAM 390
***** START SAVE SEQUENCE *****                                         EXAM 400
  2   511         0                                                     EXAM 410
  3         1  4  1  4  4   0.9   1.6   .04                             EXAM 420
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULTEXAM 430
  1   715         4         0         1         0       .20       .60    .70EXAM 440
  3                                   1         2                       EXAM 450
***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****            EXAM 460
  1   712                                               .20       .35    .40EXAM 470
  3                                   3         4                       EXAM 480
***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****             EXAM 490
  2   812                                                               EXAM 500
  3         1  4  1  4  4   0.9   1.6   .04                             EXAM 510
***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A EXAM 520
  3   906  155504   155503          0         0       .15         0   -.4EXAM 530
***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****   EXAM 540
  3   916  255504   155505          0         0       .15         0   -.4EXAM 550
***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ***4EXAM 560
  3   902  555501         0         0       1.0       .25         0    0EXAM 570
                                CUBANE                                  EXAM 580
  3  1102                                                               EXAM 590
***** END OF SAVE SEQUENCE *****                                        EXAM 600
  3   202        9.                                                     EXAM 610
***** ADVANCE PLOTTER 9 INCHES ALONG X *****                            EXAM 620
  3   503         2      -2.7                                           EXAM 630
***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****  EXAM 640
  3  1103                                                               EXAM 650
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****                EXAM 660
  3   202       20.                                                     EXAM 670
***** ADVANCE PLOTTER 20 INCHES *****                                   EXAM 680
  3   202                                                               EXAM 690
***** ADD DUMMY PLOT TO MAGNETIC TAPE *****                             EXAM 700
   -1                                                                   EXAM 710
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