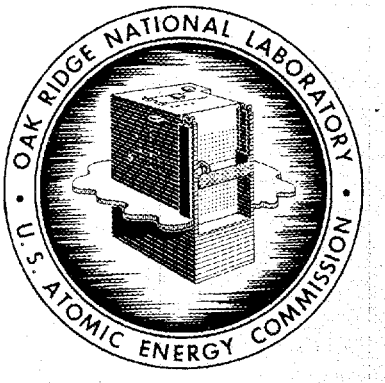

OAK RIDGE NATIONAL LABORATORY

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ORNL - TM - 305

OR FLS,

A FORTRAN CRYSTALLOGRAPHIC LEAST-SQUARES PROGRAM

W. R. Busing
K. O. Martin
H. A. Levy

NOTICE

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OR FLS,

A FORTRAN CRYSTALLOGRAPHIC LEAST-SQUARES PROGRAM

by

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CONTENTS

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	$\Sigma_i f_i a_i \exp(-T_i\rho) \Sigma_j \cos_{ij}$	$\Sigma_i f_i a_i \Sigma_j \exp_{ij} \cos_{ij}$
B	$\Sigma_i f_i a_i \exp(-T_i\rho) \Sigma_j \sin_{ij}$	$\Sigma_i f_i a_i \Sigma_j \exp_{ij} \sin_{ij}$
$\partial A/\partial f_i$	$a_i \exp(-T_i\rho) \Sigma_j \cos_{ij}$	$a_i \Sigma_j \exp_{ij} \cos_{ij}$
$\partial B/\partial f_i$	$a_i \exp(-T_i\rho) \Sigma_j \sin_{ij}$	$a_i \Sigma_j \exp_{ij} \sin_{ij}$
$\partial A/\partial a_i$	$f_i \exp(-T_i\rho) \Sigma_j \cos_{ij}$	$f_i \Sigma_j \exp_{ij} \cos_{ij}$
$\partial B/\partial a_i$	$f_i \exp(-T_i\rho) \Sigma_j \sin_{ij}$	$f_i \Sigma_j \exp_{ij} \sin_{ij}$
$\partial A/\partial T_i$	$-\rho f_i a_i \exp(-T_i\rho) \Sigma_j \cos_{ij}$	-----
$\partial B/\partial T_i$	$-\rho f_i a_i \exp(-T_i\rho) \Sigma_j \sin_{ij}$	-----
$\partial A/\partial x_i$	$-2\pi f_i a_i \exp(-T_i\rho) \Sigma_j h_j \sin_{ij}$	$-2\pi f_i a_i \Sigma_j h_j \exp_{ij} \sin_{ij}$
$\partial B/\partial x_i$	$2\pi f_i a_i \exp(-T_i\rho) \Sigma_j h_j \cos_{ij}$	$2\pi f_i a_i \Sigma_j h_j \exp_{ij} \cos_{ij}$
$\partial A/\partial B_{12i}$	-----	$-f_i a_i \Sigma_j (2hk)_j \exp_{ij} \cos_{ij}$
$\partial B/\partial \beta_{12i}$	-----	$-f_i a_i \Sigma_j (2hk)_j \exp_{ij} \sin_{ij}$

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 β_{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

$$\exp_{ij} = \exp\{-[(h^2)_j \beta^{11}_i + (k^2)_j \beta^{22}_i + (\ell^2)_j \beta^{33}_i +$$

$$(2hk)_j \beta^{12}_i + (2h\ell)_j \beta^{13}_i + (2k\ell)_j \beta^{23}_i]\}.$$

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

Rules for obtaining the transformed coefficients β^{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. **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 $P3_22$, 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. $1 \leq NS \leq 24$.*
19-21	NQ, the number of scale factors in the parameter list. $1 \leq NQ \leq 9$.*

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_{11_i}, a coefficient in the expression for the anisotropic temperature factor for atom i, $\exp[-(\beta_{11_i}h^2 + \beta_{22_i}k^2 + \beta_{33_i}\ell^2 + 2\beta_{12_i}hk + 2\beta_{13_i}h\ell + 2\beta_{23}k\ell)]$.
10-18	β_{22_i}
19-27	β_{33_i}
28-36	β_{12_i}
37-45	β_{13_i}
46-54	β_{23_i}

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) $\partial A/\partial \beta_{11\,i}$, 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-centrosymmetric structures, NS is equal to the number of equivalent positions. For centrosymmetric 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*, $\cos\alpha$*, $\cos\beta$*, $\cos\gamma$*, 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 SCREW,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,IQ,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 IQ,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(1H0,41X,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
     118X,F9.3,4X,F9.3,4X,F5.3)                                         FLS   41
00046 FORMAT(33H0WEIGHTED R FACTOR OMITTING ZEROS,                      FLS   42
     119X,F9.3,4X,F9.3,4X,F5.3)                                         FLS   43
00051 FORMAT(12A6)                                                      FLS   44
00052 FORMAT(1H1,12A6)                                                  FLS   45
00053 FORMAT(24I3)                                                      FLS   46
00054 FORMAT(32H0NUMBER OF CYCLES IN THIS JOB IS,I2/37H0NUMBER OF PARAMETFLS   47
     1ERS TO BE VARIED IS,I4)                                           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 CYCLE,I2,16H OF PREVIOUS JOBFLS   52
     1)                                                                 FLS   53
00067 FORMAT(29H0NUMBER OF PARAMETERS READ IS,I4)                       FLS   54
00068 FORMAT (I1,F8.0,7F9.0)                                            FLS   55
00069 FORMAT(31H0NUMBER OF OBSERVATIONS READ IS,I5)                     FLS   56
00070 FORMAT(72I1)                                                      FLS   57
00071 FORMAT(10F12.8)                                                   FLS   58
00072 FORMAT(46H0CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE,I2)      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/IH )                          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
     12H0SUM(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 I2/20H0SUM(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 REASONI2)                                                           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 9,00035                                     FLS  122
          GO TO 00301                                                   FLS  123
                                                                        FLS  124
00225     WRITE OUTPUT TAPE 9,00037                                     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 9,00067,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 10,00068,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 9,00069,NO                                    FLS  141
                                                                        FLS  142
C       READ KEY INTEGERS IF REFINEMENT IS TO BE MADE                   FLS  143
        IF(NC)01601,01601,01301                                         FLS  144
                                                                        FLS  145
01301      READ INPUT TAPE 10,00070,(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 9,00092                                       FLS  153
        DO 01653 I=1,NP                                                 FLS  154
                                                                        FLS  155
01653      WRITE OUTPUT TAPE 9,00093,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 02501 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
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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,C0081,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,C0041
         WRITE OUTPUT TAPE 9,C0042,RZNUM,RZDEN,RZ
         WRITE OUTPUT TAPE 9,C0043,RNUM,RZDEN,R
         WRITE OUTPUT TAPE 9,C0044,WRZNUM,WRZDEN,WRZ
         WRITE OUTPUT TAPE 9,C0046,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,C0083,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
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C                TERMINATE JOB IF SINGULAR MATRIX WAS FOUND                      FLS  301
06201            WRITE OUTPUT TAPE 9,00085                                       FLS  302
                 GO TO 11501                                                     FLS  303
                                                                                 FLS  304
                                                                                 FLS  305
C                START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR                 FLS  306
C                                                  PARAMETER CHANGES            FLS  307
06301            DO 07201 I#1,NV                                                 FLS  308
                                                                                 FLS  309
                    PDI#0.0                                                      FLS  310
                    IJ#NM-I+1                                                    FLS  311
                    IJD#NV-1                                                     FLS  312
                    DO 07001 J#1,NV                                              FLS  313
                                                                                 FLS  314
                       PDI#PDI+AM(IJ)*V(J)                                       FLS  315
                       IF(J-I)06701,06801,06901                                  FLS  316
                                                                                 FLS  317
06701                     IJ#IJ-IJD                                              FLS  318
                          IJD#IJD-1                                              FLS  319
                          GO TO 07001                                            FLS  320
                                                                                 FLS  321
C                         SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX               FLS  322
06801                     DIAG(I)#AM(IJ)                                         FLS  323
                                                                                 FLS  324
06901                     IJ#IJ-1                                                FLS  325
07001                     CONTINUE                                               FLS  326
                                                                                 FLS  327
                    PD(I)#PDI                                                    FLS  328
                    SIG#SIG-PDI*V(I)                                             FLS  329
07201               CONTINUE                                                     FLS  330
C                   END LOOP FOR MATRIX VECTOR MULTIPLICATION                    FLS  331
                                                                                 FLS  332
C                RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG                   FLS  333
                 SQSIG(I)#SQRTF(SIG/FLOATF(NO-NV))                               FLS  334
                                                                                 FLS  335
C                PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS                FLS  336
                 WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                     FLS  337
                 WRITE OUTPUT TAPE 9,00086,IC                                    FLS  338
                                                                                 FLS  339
C                START LOOP TO CORRECT AND PUT OUT PARAMETERS                    FLS  340
                 J#1                                                             FLS  341
                 N#1                                                             FLS  342
                 DO 08001 I#1,NP                                                 FLS  343
                                                                                 FLS  344
C                   SET K TO SELECT APPROPRIATE LABEL                            FLS  345
                    IF(I-NQ-1)07452,07454,07456                                  FLS  346
                                                                                 FLS  347
07452               K#1                                                          FLS  348
                    GO TO 07501                                                  FLS  349
                                                                                 FLS  350
07454               K#2                                                          FLS  351
                    GO TO 07501                                                  FLS  352
                                                                                 FLS  353
07456               IF(ITF-1)07457,07457,07461                                   FLS  354
                                                                                 FLS  355
07457                  K#XMODF(I-NQ-2,6)+3                                       FLS  356
                       IF(K-8)07462,07459,07459                                  FLS  357
                                                                                 FLS  358
07459                     K#14                                                   FLS  359
                          GO TO 07501                                            FLS  360
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                                                                      FLS  361
07461                      K#XMODF(I-NQ+2,11)+3                       FLS  362
                                                                      FLS  363
07462                IF(K-3)07501,07463,07501                         FLS  364
                                                                      FLS  365
07463                   WRITE OUTPUT TAPE 9,00078,ATOM(N)             FLS  366
                        N#N+1                                         FLS  367
                                                                      FLS  368
C                    TEST KEY INTEGERS                                FLS  369
07501                IF(K1(I))07601,07601,07701                       FLS  370
                                                                      FLS  371
07601                   WRITE OUTPUT TAPE 9,00088,(LABEL(L,K),L#1,2),  FLS  372
     1                                                P(I),P(I)        FLS  373
                        GO TO 08001                                   FLS  374
                                                                      FLS  375
07701                   POLD#P(I)                                     FLS  376
                        P(I)#POLD+PD(J)                               FLS  377
                        SIGP#SQRTF(DIAG(J))*SQSIG(1)                  FLS  378
                        WRITE OUTPUT TAPE 9,00089,(LABEL(L,K),L#1,2),  FLS  379
     1                                          POLD,PD(J),P(I),SIGP  FLS  380
                        J#J+1                                         FLS  381
                                                                      FLS  382
08001                CONTINUE                                         FLS  383
C                    END LOOP TO CORRECT AND PUT OUT PARAMETERS       FLS  384
                                                                      FLS  385
C                 PUT OUT ESTIMATED AGREEMENT FACTORS                 FLS  386
                  WRITE OUTPUT TAPE 9,00081,IC,SIG,SQSIG(1)           FLS  387
                                                                      FLS  388
C                 ENTER SUBROUTINE TO TEST PARAMETERS                 FLS  389
                  ISTOP#0                                             FLS  390
                  CALL TEST                                           FLS  391
                                                                      FLS  392
C                 WRITE CORRECTED PARAMETERS ON AUXILIARY TAPE IF     FLS  393
C                                                    DESIRED          FLS  394
08201             IF(IT)08202,08301,08202                             FLS  395
                                                                      FLS  396
08202                NT#IT+4                                          FLS  397
                     NPCD#8*((NQ-1)/8+1)                              FLS  398
                     WRITE OUTPUT TAPE NT,00031,(SC(I),I#1,NPCD)      FLS  399
                     WRITE OUTPUT TAPE NT,00032,TO                    FLS  400
                     DO 08209 I#1,NA                                  FLS  401
                                                                      FLS  402
                        WRITE OUTPUT TAPE NT,00033,ATOM(I),SF(I),A1(I), FLS  403
     1                                              (XYZ(K,I),K#1,3)  FLS  404
08209                   WRITE OUTPUT TAPE NT,00034,(BETA(K,I),K#1,6)  FLS  405
                                                                      FLS  406
C                 TERMINATE JOB IF INDICATED BY USERS SUBROUTINE TEST FLS  407
08301             IF(ISTOP)08401,08501,08401                          FLS  408
                                                                      FLS  409
08401                WRITE OUTPUT TAPE 9,00090,ISTOP                  FLS  410
                     GO TO 08701                                      FLS  411
                                                                      FLS  412
08501                CONTINUE                                         FLS  413
C                    END LOOP THROUGH NC CYCLES AND FINAL CALC OF Y   FLS  414
                                                                      FLS  415
C     TERMINATE JOB                                                   FLS  416
08701 IF(NC)11701,11701,08801                                         FLS  417
                                                                      FLS  418
C        CALCULATE AND PUT OUT CORRELATION MATRIX                     FLS  419
08801    WRITE OUTPUT TAPE 9,00052,(TITLE(I),I#1,12)                  FLS  420
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```
      WRITE OUTPUT TAPE 9,CC097                                          FLS  421
      DO 09101 I#1,NV                                                    FLS  422
                                                                         FLS  423
         DIAG(I)#1.0/SQRTF(DIAG(I))                                      FLS  424
09101    CONTINUE                                                        FLS  425
                                                                         FLS  426
      IJ#NM                                                              FLS  427
      DO 10201 I#1,NV                                                    FLS  428
                                                                         FLS  429
         DO 09601 J#I,NV                                                 FLS  430
                                                                         FLS  431
            ROW(J)#0.0                                                   FLS  432
09601       CONTINUE                                                     FLS  433
                                                                         FLS  434
         DO 10001 J#I,NV                                                 FLS  435
                                                                         FLS  436
            ROW(J)#AM(IJ)*DIAG(I)*DIAG(J)                                FLS  437
            IJ#IJ-1                                                      FLS  438
10001       CONTINUE                                                     FLS  439
                                                                         FLS  440
         WRITE OUTPUT TAPE 9,CCC98,I,(ROW(J),J#I,NV)                     FLS  441
10201    CONTINUE                                                        FLS  442
                                                                         FLS  443
C     WRITE DATA REQUIRED FOR FUNCTION AND ERROR PROGRAM                 FLS  444
10501 IF(IXFE)10601,11501,10601                                          FLS  445
                                                                         FLS  446
10601    WRITE OUTPUT TAPE 3,CC053,ITF,NO,NP                             FLS  447
         WRITE OUTPUT TAPE 3,CC071,(P(I),I#1,NP)                         FLS  448
         WRITE OUTPUT TAPE 3,CC07C,(K(I),I#1,NP)                         FLS  449
         WRITE OUTPUT TAPE 3,CC053,NV                                    FLS  450
                                                                         FLS  451
         VARI#SQSIG(1)**2                                                FLS  452
         DO 10703 I#1,NM                                                 FLS  453
                                                                         FLS  454
10703       AM(I)#AM(I)*VARI                                             FLS  455
                                                                         FLS  456
         K#NM/2                                                          FLS  457
         L#NM                                                            FLS  458
         DO 11201 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
11201       CONTINUE                                                     FLS  465
                                                                         FLS  466
         WRITE OUTPUT TAPE 3,CC099,(AM(I),I#1,NM)                        FLS  467
         END FILE 3                                                      FLS  468
11501 IF(IT-1)11701,11601,11701                                          FLS  469
                                                                         FLS  470
11601    END FILE 5                                                      FLS  471
                                                                         FLS  472
11701 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
```

```
                                                                      FLS  478
      SUBROUTINE PRELIM                                               FLS  479
                                                                      FLS  480
      COMMON NC,NV,NX,IW,IP,IT,NP,ISENT,NO,NM,NCY,IC,SIG,YC           FLS  481
      COMMON SQRTW,DY,WDY,JK,ISING,II,IID,PDI,IJ,IJD,POLD             FLS  482
      COMMON SIGP,ISTOP,NT,NPCD,IXFE,HOLD,VARI                        FLS  483
      COMMON TITLE,P,X,YO,SIGYO,KI,SQSIG,AM,V,DC,DV,DIAG,PD,ROW       FLS  484
      COMMON RNUM,RZNUM,RZDEN,WRNUM,WRZNUM,WRZDEN,R,RZ,WR,WRZ         FLS  485
      COMMON LABEL,ATOM,IHKL                                          FLS  486
      COMMON IFSQ,ITF,NF,NA,ICENT,NS,NQ,TO,TJ,HX,HHB,EXPIJ,COSIJ,SINIJ FLS  487
      COMMON FI,A,B,RHO,SINTHL,PT,IPT,FRACPT,FTA,FTACOS,FTASIN,TFI,PIFI FLS  488
      COMMON IQ,SQTO,SQRTAB,F,DFDTO                                   FLS  489
      COMMON SC,SF,AI,XYZ,BETA,DADFI,DBDFI,DADAI,DBDAI,DADX,DBDX,DADB FLS  490
      COMMON DBDB,DFDS,DFDFI,DFDAI,DFDX,DFDB,TS,IS,HJ,HHJ,RCP,FX,PRCP FLS  491
      COMMON CA,CB                                                    FLS  492
                                                                      FLS  493
C     DIMENSIONS FOR NV(MAX)#100,NP(MAX)#230,NO(MAX)#2500,NX(MAX)#4,  FLS  494
C        NF(MAX)#10,NA(MAX)#20,NS(MAX)#24,NQ(MAX)#9                   FLS  495
      DIMENSION TITLE(12),P(230),X(4,2500),YO(2500),SIGYO(2500),KI(230) FLS 496
      DIMENSION SQSIG(2),AM(5150),V(100),DC(230),DV(100)              FLS  497
      DIMENSION DIAG(100),PD(100),ROW(100),ATOM(20),LABEL(2,14),IHKL(4) FLS 498
      DIMENSION SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20),DADFI(20)   FLS  499
      DIMENSION DBDFI(20),DADAI(20),DBDAI(20),DADX(4,20),DBDX(3,20)   FLS  500
      DIMENSION DADB(6,20),DBDB(6,20),DFDS( 9),DFDFI(20),DFDAI(20)    FLS  501
      DIMENSION DFDX(3,20),DFDB(6,20),TS(4,24),IS(2,3,24),HJ(3),H(4)  FLS  502
      DIMENSION HHJ(6),RCP(6),FX(32,10),PRCP(6)                       FLS  503
                                                                      FLS  504
C     READ AND PUT OUT CONTROL INFORMATION                            FLS  505
      READ INPUT TAPE 10,2,IFSQ,ITF,NF,NA,ICENT,NS,NQ                 FLS  506
    2 FORMAT (7I3)                                                    FLS  507
      IF(IFSQ-1)4,4,7                                                 FLS  508
                                                                      FLS  509
    4    WRITE OUTPUT TAPE 9,5                                        FLS  510
    5    FORMAT (1H0BASED ON F)                                       FLS  511
         GO TO 9                                                      FLS  512
                                                                      FLS  513
    7    WRITE OUTPUT TAPE 9,8                                        FLS  514
    8    FORMAT (19H0BASED ON F SQUARED)                              FLS  515
                                                                      FLS  516
    9 IF(ITF-2)10,13,16                                               FLS  517
                                                                      FLS  518
   10    WRITE OUTPUT TAPE 9,11                                       FLS  519
   11    FORMAT (30H0ISOTROPIC TEMPERATURE FACTORS)                   FLS  520
         GO TO 19                                                     FLS  521
                                                                      FLS  522
   13    WRITE OUTPUT TAPE 9,14                                       FLS  523
   14    FORMAT (32H0ANISOTROPIC TEMPERATURE FACTORS)                 FLS  524
         GO TO 19                                                     FLS  525
                                                                      FLS  526
   16    WRITE OUTPUT TAPE 9,17                                       FLS  527
   17    FORMAT (43H0ISOTROPIC TEMPERATURE FACTORS CONVERTED TO,      FLS  528
     1      28H ANISOTROPIC BEFORE REFINING)                          FLS  529
                                                                      FLS  530
   19 WRITE OUTPUT TAPE 9,20,NF                                       FLS  531
   20 FORMAT (38H0NUMBER OF SCATTERING FACTOR TABLES IS I3)           FLS  532
      WRITE OUTPUT TAPE 9,22,NA                                       FLS  533
   22 FORMAT (38H0NUMBER OF ATOMS IN ASYMMETRIC UNIT IS I3)           FLS  534
      IF(ICENT-1)24,24,27                                             FLS  535
                                                                      FLS  536
   24    WRITE OUTPUT TAPE 9,25                                       FLS  537
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   25    FORMAT (16HOCENTROSYMMETRIC)                                      FLS  538
         GO TO 29                                                          FLS  539
                                                                           FLS  540
   27    WRITE OUTPUT TAPE 9,28                                            FLS  541
   28    FORMAT (20HONON-CENTROSYMMETRIC)                                  FLS  542
                                                                           FLS  543
   29 WRITE OUTPUT TAPE 9,30,NS                                            FLS  544
   30 FORMAT (28HONUMBER OF SYMMETRY CARDS IS I3)                          FLS  545
      WRITE OUTPUT TAPE 9,32,NQ                                            FLS  546
   32 FORMAT (27HONUMBER 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 (24HOSCATTERING 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(I,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 (21HOSYMMETRY INFORMATION/67HO     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 (29HORECIPROCAL 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
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      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*PROP(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,VAR1                           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,PI,IPI,FRACPI,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(2,4),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)
```

```
                                                                      FLS  715
C       START LOOP THROUGH THE NA ATOMS                               FLS  716
        DO 2201 I#1,NA                                                FLS  717
                                                                      FLS  718
C          ENTER USERS SUBROUTINE TO SET INDICES FOR SPECIAL POSITIONS FLS  719
           CALL PATCH(I,TJ,HJ,HHJ)                                    FLS  720
                                                                      FLS  721
C          COMPUTE TRIGONOMETRIC TERMS                                FLS  722
           HX#TJ                                                      FLS  723
           DO 603 K#1,3                                               FLS  724
                                                                      FLS  725
  603         HX#HX+HJ(K)*XYZ(K,I)                                    FLS  726
                                                                      FLS  727
           COSIJ#COSF(6.2831853*HX)                                   FLS  728
           SINIJ#SINF(6.2831853*HX)                                   FLS  729
                                                                      FLS  730
C          COMPUTE ANISOTROPIC TEMPERATURE FACTOR                     FLS  731
           IF(ITF-1)901,901,801                                       FLS  732
                                                                      FLS  733
  801      HHB#0.0                                                    FLS  734
           DO 803 K#1,6                                               FLS  735
                                                                      FLS  736
  803         HHB#HHB+HHJ(K)*BETA(K,I)                                FLS  737
                                                                      FLS  738
           EXPIJ#EXPF(-HHB)                                           FLS  739
           COSIJ#COSIJ*EXPIJ                                          FLS  740
           SINIJ#SINIJ*EXPIJ                                          FLS  741
                                                                      FLS  742
C          ACCUMULATE REQUIRED SUMS                                   FLS  743
  901      DADFI(I)#DADFI(I)+COSIJ                                    FLS  744
           DO 1101 K#1,3                                              FLS  745
                                                                      FLS  746
 1101         DADX(K,I)#DADX(K,I)+HJ(K)*SINIJ                         FLS  747
                                                                      FLS  748
           IF(ITF-1)1501,1501,1301                                    FLS  749
                                                                      FLS  750
 1301      DO 1401 K#1,6                                              FLS  751
                                                                      FLS  752
 1401         DADB(K,I)#DADB(K,I)+HHJ(K)*COSIJ                        FLS  753
                                                                      FLS  754
C          BYPASS REMAINING SUMS IF CENTROSYMMETRIC                   FLS  755
 1501      IF(ICENT-1)2201,2201,1601                                  FLS  756
                                                                      FLS  757
 1601      DBDFI(I)#DBDFI(I)+SINIJ                                    FLS  758
           DO 1801 K#1,3                                              FLS  759
                                                                      FLS  760
 1801         DBDX(K,I)#DBDX(K,I)+HJ(K)*COSIJ                         FLS  761
                                                                      FLS  762
           IF(ITF-1)2201,2201,2001                                    FLS  763
                                                                      FLS  764
 2001      DO 2101 K#1,6                                              FLS  765
                                                                      FLS  766
 2101         DBDB(K,I)#DBDB(K,I)+HHJ(K)*SINIJ                        FLS  767
                                                                      FLS  768
 2201      CONTINUE                                                   FLS  769
C          END LOOP THROUGH THE NA ATOMS                              FLS  770
                                                                      FLS  771
 2301   CONTINUE                                                      FLS  772
C       END LOOP THROUGH THE NS SYMMETRY TRANSFORMATIONS              FLS  773
                                                                      FLS  774
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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(1,I)*RHO)                                        FLS  806
                                                                             FLS  807
C        COMPUTE A AND ITS DERIVATIVES                                       FLS  808
 3501    FTA=FI*TFI*AI(I)                                                    FLS  809
         FTACOS=FTA*DACFI(I)                                                 FLS  810
         A=A+FTACOS                                                          FLS  811
         DACAI(I)=FI*TFI*DACFI(I)                                            FLS  812
         DACFI(I)=AI(I)*TFI*DACFI(I)                                         FLS  813
         PIFI=-6.28318531*FTA                                                FLS  814
         DO 3801 K=1,3                                                       FLS  815
                                                                             FLS  816
 3801       DACX(K,I)=PIFI*DACX(K,I)                                        FLS  817
                                                                             FLS  818
         IF(ITF-1)4201,4201,4101                                             FLS  819
                                                                             FLS  820
 4101    DO 4101 K=1,6                                                       FLS  821
                                                                             FLS  822
 4101       DACB(K,I)=-FTA*DACB(K,I)                                        FLS  823
                                                                             FLS  824
            GO TO 4301                                                       FLS  825
                                                                             FLS  826
 4201       DACB(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
```

```
      DBCFI(I)=AI(I)*TFI*DBDFI(I)                                       FLS  835
      PIFI=-PIFI                                                        FLS  836
      DO 4701 K=1,3                                                     FLS  837
                                                                        FLS  838
 4701    DBCX(K,I)=PIFI*DBCX(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       DBCB(K,I)=-FTA*DBCB(K,1)                                    FLS  845
                                                                        FLS  846
            GO TO 5201                                                  FLS  847
                                                                        FLS  848
 5101       DBCB(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=5(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  882
                                                                        FLS  883
 5901    DFDS(IQ)=F/SC(IQ)                                              FLS  884
 5902    DFDTO=-RHO*F                                                   FLS  885
         GO TO 6501                                                     FLS  886
                                                                        FLS  887
 6001    SQTO=SQTO**2                                                   FLS  888
         IF(ICENT-1)6201,6201,6301                                      FLS  889
                                                                        FLS  890
 6201       CA=8.0*SQTO*A                                               FLS  891
            CB=0.0                                                      FLS  892
            F=CA*A/2.0
```

```
            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(I,1)#CA*DADB(I,I)+CB*DBDB(I,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 SBTOPIDER,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,PCLO                  FLS  937
       COMMON SIGP,ISIGP,NT,NPCD,IXFE,HOLD,VARI                             FLS  938
       COMMON TITLE,P,X,YO,SIGYO,KI,SQSIG,AM,V,DC,CV,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
```

```
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 SOSIG(2),AM(5150),V(100),DC(230),DV(100)                     FLS  951
      DIMENSION DIAG(300),PD(100),ROW(100),ATOM(20),LABEL(2,24),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(5,24),IS(2,3,24),HJI(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(2PHOTEMPERATURE FACTOR OF ATOM I2,                           FLS 1006
     1      25H IS NOT POSITIVE-DEFINITE)                                    FLS 1007
         ISTOP#1                                                             FLS 1008
```

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                                                                        FLS 1009
  220    CONTINUE                                                       FLS 1010
C        END LOOP THROUGH NA ATOMS                                      FLS 1011
                                                                        FLS 1012
       TO#0.0                                                           FLS 1013
                                                                        FLS 1014
C      COPY PARAMETERS INTO THE ARRAY P                                 FLS 1015
       CALL SBTOP(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)                  FLS 1016
       RETURN                                                           FLS 1017
       END                                                              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
```

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      SUBROUTINE SBTOP(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NQ,NP)              FLS 1063
      DIMENSION P(230),SC( 9),SF(20),AI(20),XYZ(3,20),BETA(6,20)         FLS 1064
                                                                         FLS 1065
   10 I#1                                                                FLS 1066
   20 DO 40 J#1,NQ                                                       FLS 1067
                                                                         FLS 1068
   30    P(I)#SC(J)                                                      FLS 1069
   40    I#I+1                                                           FLS 1070
                                                                         FLS 1071
   50 P(I)#TO                                                            FLS 1072
   60 I#I+1                                                              FLS 1073
   70 DO 220 J#1,NA                                                      FLS 1074
                                                                         FLS 1075
   80    P(I)#SF(J)                                                      FLS 1076
   90    P(I+1)#AI(J)                                                    FLS 1077
  100    I#I+2                                                           FLS 1078
  110    DO 130 K#1,3                                                    FLS 1079
                                                                         FLS 1080
  120       P(I)#XYZ(K,J)                                                FLS 1081
  130       I#I+1                                                        FLS 1082
                                                                         FLS 1083
  140    IF(ITF-1)150,150,190                                            FLS 1084
                                                                         FLS 1085
  150       P(I)#BETA(1,J)                                               FLS 1086
  160       I#I+1                                                        FLS 1087
  170       GO TO 220                                                    FLS 1088
                                                                         FLS 1089
  190       DO 210 K#1,6                                                 FLS 1090
                                                                         FLS 1091
  200          P(I)#BETA(K,J)                                            FLS 1092
  210          I#I+1                                                     FLS 1093
                                                                         FLS 1094
  220    CONTINUE                                                        FLS 1095
                                                                         FLS 1096
      RETURN                                                             FLS 1097
      END                                                                FLS 1098


*TYPE(FAP)                                                               FLS 1099
       COUNT   230                                                       FLS 1100
       REM SYMMETRIC MATRIX INVERSE. SEE GLOSSARY FOR STORAGE SCHEME.    FLS 1101
       REM FOR USE ON 704, 709, OR 7090.                                 FLS 1102
       REM WRITTEN IN FAP FOR ASSEMBLY ON 709 OR 7090.                   FLS 1103
       ENTRY   SMI                                                       FLS 1104
 SMI   SXD T13,1                                                         FLS 1105
       SXD T14,2                                                         FLS 1106
       LFTM                                                              FLS 1107
       TNO *+1                          OVERFLOW TOGGLES                 FLS 1108
       CAL 1,4                                                           FLS 1109
       COM                                                               FLS 1110
       PAX 0,2                                                           FLS 1111
       TXI *+1,2,1                                                       FLS 1112
       CLA 2,4                                                           FLS 1113
       STA Y1                                                            FLS 1114
       CLA 3,4                                                           FLS 1115
       STA Y28                                                           FLS 1116
       STA SING1                                                         FLS 1117
 Y1    CLA 0                      ADD SET                                FLS 1118
       PDX 0,1                                                           FLS 1119
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        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 PON                 Y14                              FLS 1156
        SUB T3                                                   FLS 1157
        ARS 18                                                   FLS 1158
        STA Y16A                     SETS ADDRESSES              FLS 1159
        STA Y19                         AT M                     FLS 1160
        CLA PON                                                  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 OFL,4                                                FLS 1177
        LXD T12,4                                                FLS 1178
Y16A    STO 0,1                      ADD SET Y14,M               FLS 1179
```

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DTI   TNX Y15,0,0                    DEC FOR TI,C(14)                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
      TNC Y19C                                                       FLS 1191
      SXD T12,4                                                      FLS 1192
      TSX OFL,4                                                      FLS 1193
      LXD T12,4                                                      FLS 1194
Y19C  STQ 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
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        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
DTI2    TNX Y26,0,0                  DEC FOR TI2                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
   O            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     18C.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      1C.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      1C.8                         1                         FLS 1469
1                                                                                              FLS 1470
1000111111111100100101110                                                                      FLS 1471
```

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       2.106       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
```

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	143.8837	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

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	-18.1159	-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	-8.3646	-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	13.2928	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

SQRT(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
2	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	-6.8145	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	33.5000	30.3763	1.8161	-2.6591	3.1237	1.0000	3.1237	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	5.9913	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	3	-3	233.3000	231.6780	-8.0738	-12.8968	-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	9.2940	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	3	7	10.6000	13.9148	3.3502	-0.8260	-3.3148	1.0000	-3.3148	1
1	3	-7	78.0000	75.7974	-1.6880	-8.3378	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	3	-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 02

SQRT(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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