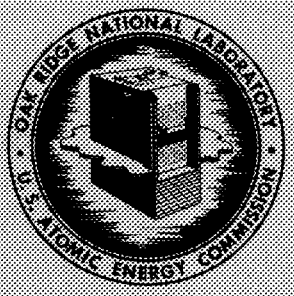

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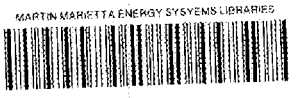

ORNL-TM-306

10

OR FFE,

A FORTRAN CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM

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

ORNL-TM-306

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by

W. R. Busing, K. O. Martin, and H. A. Levy
Chemistry Division and Mathematics Division

MARCH 1964

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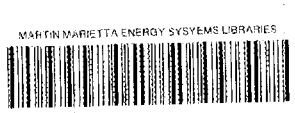

CONTENTS

ABSTRACT

This report describes a computer program which calculates interatomic distances, bond angles, principal axes of thermal motion, and other functions of the unit cell parameters, the atomic coordinates, and the temperature factor coefficients of a crystal structure. The standard errors of these functions are computed from the variance-covariance matrix of the parameters if this is known. The program may be used independently, or the input may be taken from a magnetic tape prepared by the crystallographic least-squares program OR FLS.

The program is written entirely in Fortran, and detailed instructions for its use are included. The necessary card decks may be obtained from the authors.

INTRODUCTION

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

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

will be given below together with detailed specifications for writing subroutines for new functions.

This program is a revision of the earlier OR XFE (W. R. Busing and H. A. Levy, "A Crystallographic Function and Error Program for the IBM 704," ORNL-CF 59-12-3 (1959)). It is now written entirely in Fortran II and comments have been added to facilitate any modification which may be desired. Card decks are available from the authors on request.

MATHEMATICAL METHOD

The functions which the program computes are of the form

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

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

The standard error of f is given by

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

where

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

and

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

Here V_{ij} is an element of the variance-covariance matrix which describes the errors of the atomic parameters, and U_{ij} is an element of a similar matrix for the unit cell parameters. $C_{ij} = 1$ if $i = j$; otherwise $C_{ij} = 2$.

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

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

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

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

$$U_{ii} = \sigma^2(a_i)$$

$$U_{ij} = 0, \quad i \neq j.$$

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

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

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

The increment used is $\Delta p_i = (0.01)V_{ii}^{1/2}$. The derivatives

with respect to the cell parameters are obtained similarly.

The program is arranged so that it computes derivatives only with respect to the parameters actually involved in f. The information as to which these are is provided by the subroutines PRE1, PRE2, etc., which are supplied for each type of function. Derivative computations are also omitted with respect to fixed parameters which are not represented in the variance-covariance matrix. If this situation arises because certain atoms are in special positions, then the errors are computed correctly. However, if parameters have been fixed for other reasons, it is possible that important terms are omitted from the calculated errors.

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

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

CONSTRAINTS ON THE PARAMETERS

In order to insure that this program correctly computes the errors of various functions, it is necessary for the user to consider whether the symmetry of the crystal introduces constraints either on the cell parameters, a_i, or on the atomic parameters, p_i. A simple case occurs when the symmetry forces a parameter to have a fixed value, and this situation is correctly treated by specifying that the error of this parameter is zero. A more complicated procedure is required when the symmetry imposes a relationship between two or more parameters. In this case one of the interrelated parameters is chosen as independent and a Fortran II subroutine is written to set the values of the dependent parameters in terms of it. The main program will enter this subroutine immediately before each entry to the function-computing subroutine so that the derivatives needed for the error calculation are correctly computed. In the input data the errors associated with the dependent parameters should be set to zero. (When the atomic parameters are taken from a least-squares refinement these errors are automatically zero, since the dependent parameters would not have been varied.)

Specifications are given here for subroutines SETA and SETP which establish these constraints, and examples are included in the sample calculations. The statements required are summarized as follows:

```
SUBROUTINE SETA(A)
DIMENSION A(6)
Include statements to set the values of the A(I)'s
which are taken as dependent in terms of those chosen
as independent.
RETURN
END
SUBROUTINE SETP(P)
DIMENSION P(300)
Include statements to set the values of the P(I)'s
which are taken as dependent in terms of those chosen
as independent.
RETURN
END
```

These routines should be compiled and substituted in the binary deck for the dummy routines with the same names.

ATOM DESIGNATION AND SYMMETRY TRANSFORMATIONS

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

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

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

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

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

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

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

For example, atom (3,208) is atom 3 in the parameter list transformed to symmetry position 8 of cell 2, while atom (5,0) is atom 5 just as it appears in the list of parameters. In a subsequent section we will refer to atom 3 in asymmetric unit 208 or atom 5 in the basic asymmetric unit (unit 0).

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

The program obtains the matrix of the anisotropic temperature factor coefficients of an atom in a similar way except that the elements of this matrix are transformed as the corresponding products of the coordinates. This procedure is valid for an atom in either a special or general position provided that the symmetry cards are written for general positions. (See H. A. Levy, Acta Cryst. (1956). 9, 679). The translational part of the symmetry transformation is irrelevant in this case as is the cell translation c. If a = 0, a null matrix will be generated.

DATA INPUT

1. Title card. FORMAT(12A6)

Columns	
1-72	Title consisting of any desired Hollerith information. This will be printed unchanged on the output.

2. Control card. FORMAT(9I3)

Columns	
1-3	IPM, the atomic parameter error indicator. The variance-covariance matrix and parameter selection information will (IPM = 0) not be used. (IPM = 1) be used to compute errors.
4-6	NP, the input indicator. If NP = 0, the structure parameters will be read from the private tape written by OR FLS. (If the variance-covariance matrix and parameter selection information are to be used, they will also be read from this tape when NP = 0). If NP > 0, data will be taken entirely from cards, and NP is equal to the number of structure parameters to be read from the cards. $0 \leqslant NP \leqslant 300$.

Columns

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

10-12 NS, the number of symmetry cards to be read.
$0 \leqslant NS \leqslant 48$.

13-15 NV, the order of the variance-covariance matrix, PM, if it is to be read from cards. If the matrix is to be read from the OR FLS tape, NV will also be read from this tape and this field is irrelevant. If the variance-covariance matrix is not to be used, set NV = 0.
$0 \leqslant NV \leqslant 200$.

The following parameter arrangement integers must be supplied if the structure parameters are read from cards. They are supplied automatically by the program if the parameters are read from the private output tape of OR FLS. For more details see 3 below.

Columns

16-18 JXP, the period of the position parameters in the parameter list. If no position parameters are included in the list, set JXP and JX = 0.

19-21 JX, the position of the first x coordinate in the parameter list.

22-24 JBP, the period of the temperature factor coefficients in the parameter list. If no temperature factor coefficients are included in the list, set JBP and JB = 0.

25-27 JB, the position of the first temperature factor coefficient in the parameter list.

3. Atomic parameter cards. FORMAT(8F9.4)
If NP = 0, the atomic parameters will be read from the private output tape of OR FLS, and the atomic parameter cards are omitted from the card input. Otherwise NP parameters must be punched eight per card. The arrangement of these parameters is subject to the following restrictions:

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

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

c) If anisotropic temperature factor coefficients are included, they must be in the sequence β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}, for each atom. These β's are defined by the following expression for the temperature factor:

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

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

Thus the position parameters of atom I start with P(J) where J = JXP*(I-1) + JX, and the temperature factor coefficients of atom I start with P(K) where K = JBP*(I-1) + JB.

4. Parameter selection cards. FORMAT(72I1)
The purpose of these cards is to identify those parameters which are associated with the elements of the variance-covariance matrix PM. They are exactly the same as the parameter selection cards used with OR FLS.

These cards are not to be supplied unless the control card integers IPM and NP specify that the variance-covariance matrix and parameter selection information will be used and will be read from cards (IPM = 1 and NP > 0).

Each column of a parameter selection card corresponds to one parameter. The first card is associated with parameters 1 to 72, the second with parameters 73 to 144, etc. If a parameter is represented in the matrix a one is punched in the corresponding column; otherwise a zero or blank is punched. The total number of one punches must be equal to NV, the order of the matrix. The first parameter in the list for which a one punch is found is assumed to correspond to the first row and column of the matrix, the second with the second, etc.

5. Variance-covariance matrix, PM, for structure parameters. FORMAT(6E12.6)
These cards are to be supplied only if the variance-covariance matrix is to be used and is to be read from cards (IPM = 1 and NP > 0).

First card
Columns

1-12 A scale factor by which the matrix will be multiplied. This could be unity or $\Sigma w(F_o - F_c)^2/(m - n)$, for example.

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

6. Cell parameter card. FORMAT(6F9.4)
These six direct unit cell parameters must always be supplied.

Columns

1-9 A(1) = a

10-18 A(2) = b

19-27 A(3) = c

28-36 A(4) = cos α

37-45 A(5) = cos β

46-54 A(6) = cos γ

7. Cell parameter error cards.
If the effect of the cell parameter errors is not to be considered (IAM = 0), these cards are omitted. If it is to be included, the cell parameter errors must be supplied in one of two forms as specified by the control card integer IAM.

a) Standard error form (IAM = 1). FORMAT(6F9.4)
If this input is used the covariances between the cell parameters are assumed to be zero.

Columns

1-9 σ(a)

10-18 σ(b)

19-27 σ(c)

28-36 σ(cos α)

37-45 σ(cos β)

46-54 σ(cos γ)

b) Variance-covariance matrix form (IAM = 2). If information on the covariances between cell parameters is available, the 21 unique elements of this 6 x 6 matrix should be punched on three cards.

FORMAT(8F9.4)

Card 1: AM(a,a), AM(a,b),...., AM(a, cos γ), AM(b,b), AM(b,c).
Card 2: AM(b, cos α),...., AM(b, cos γ), AM(c,c),...., AM(cos α, cos α).
Card 3: AM(cos α, cos β),...., AM(cos γ, cos γ).

8. Symmetry cards. FORMAT(F11.6,2I2,F11.6,2I2,F11.6,2I2) The number of symmetry cards to be read is given by NS on the control card. There must be a card for each symmetry transformation which will be called for by an instruction card (see the section "Atom Designation and Symmetry Transformations"). If the functions to be computed require no symmetry transformations, then no symmetry cards need be supplied.

These symmetry cards have the same format as those for **OR FLS**.

Columns	
1-11	Translational part of x_j or blank.
12-13	1, 2, 3, -1, -2, -3, or blank for x, y, z, -x, -y, -z, or blank, respectively, as used in the expression for the transformed x_j.
14-15	1, 2, 3, -1, -2, -3, or blank for x, y, z, -x, -y, -z, or blank, respectively, as used in the expression for the transformed x_j. (Columns 12 and 13 are exactly equivalent to 14 and 15. Also, note that an expression such as x_j = 2x must be treated as x_j = x + x.)
16-26	Translational part of y_j or blank.
27-30	Integers representing plus or minus x, y, or z in the expression for the transformed y_j as described above.
31-41	Translational part of z_j or blank.
42-45	Integers representing plus or minus x, y, or z in the expression for the transformed z_j.

9. Instruction cards. FORMAT(24I3)
   See the next section, "Instruction Input," for the specifications for this input.

10. Instruction termination card. FORMAT(24I3)
    Columns
    1-3 0 (zero) as a sentinel for the end of the instruction deck.

INSTRUCTION INPUT

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

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

Function 1

One interatomic distance.

Columns

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

Function 101

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

Columns

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

Function 201

All distances (less than d(max)) between atoms in the basic asymmetric unit and atoms in all asymmetric units (i.e., all combinations of c and s).

In order to cause this instruction to compute all possible distances less than d(max), the basic asymmetric unit should be chosen close to the origin, and the symmetry transformations specified should generate asymmetric units to fill out a unit cell on the positive sides of this basic unit. Even so, for certain symmetry situations or for small unit cells, some of the desired distances will be omitted if the atoms involved lie outside of the eight unit cells

generated. The user may prefer to use instruction 101 and to select in advance the asymmetric units likely to be involved in these contacts.

Columns

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

Function 2

Angle defined by three atoms.

Columns

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

Function 3

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

Columns

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

Function 4

Difference between two interatomic distances.

Columns

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

Function 5

Difference between two angles each defined by three atoms.

Columns

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

Function 6

The sum of several angles each defined by three atoms.

Columns

1-3	6	
4-6	n, the number of angles to be summed.	
7-12	Atom designation 1	Angle 1
13-18	Atom designation 2 (vertex)	
19-24	Atom designation 3	

Columns

25-30	Atom designation 4	
31-36	Atom designation 5 (vertex)	Angle 2
37-42	Atom designation 6	
	etc.	

Function 7

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

Columns

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

Function 107

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

Columns

1-3	107
4-9	Atom designation

Function 207

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

Columns

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

Function 8

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

Columns

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

Function 108

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

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

Function 208

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

Columns

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

Function 9

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

Columns

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

Function 109

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

Columns

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

Function 209

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

Columns

1-3	209
4-6	a(max), the number of atoms in the parameter list.
7-9	Designation of the asymmetric unit.
10-12	---

Columns

13-18	Atom designation 2	Vector
19-24	Atom designation 3	

Function 10

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

Columns

1-3	10		
4-9	Atom designation 1		
10-12	r (= 1, 2, or 3)		
13-15	i (= 1, 2, or 3)		
16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 110

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

Columns

1-3	110
4-9	Atom designation 1
10-15	---

Columns

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

Function 210

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

Columns

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

Function 11

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

Columns

1-3	11
4-9	Atom designation 1
10-12	r (= 1, 2, or 3)

Columns

13-15	i (= 1, 2, or 3)		
16-21	Atom designation 2	Vector	Vectors defining axes
22-27	Atom designation 3		
28-33	Atom designation 4	Vector	
34-39	Atom designation 5		

Function 111

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

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

Function 211

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

Columns

1-3	211
4-6	a(max), the number of atoms in the parameter list.
7-9	Designation of asymmetric unit.
10-15	---

Columns

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

Function 12

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

Columns

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

Function 13

The RMS radial thermal displacement of an atom.

Columns

1-3	13
4-9	Atom designation

Function 14

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

Columns

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

Function 15

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

Columns

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

TAPES REQUIRED

Listed here are the monitor control cards required for operation at the Oak Ridge Central Data Processing Facility. At other installations the necessary tapes should be specified appropriately.

*TAPE(3, Reel Number, SAVE)

This tape is required only if NP = 0, indicating that information is to be taken from the output of OR FLS. It will be rewound before being read and may be file protected if desired.

*TAPE(9, OUTPUT)

This is the monitor output tape to be listed.

*TAPE(10, INPUT)

This is the monitor input tape prepared from cards.

ERROR INDICATORS

If an error is detected in the course of computing a function, an indicator is put out in place of the result, and the program proceeds to compute the next function. The form of the indicator is "***NG" where NG is an integer, the meaning of which is tabulated here.

NG	Subprogram	Meaning
1	ATOM, BETA	The symmetry position specified is out of range of the symmetry cards supplied.
4	BETA	The temperature factors are not in anisotropic form. Either ITF = 1 on OR FLS tape or JBP $<$ 6 when parameters are read from cards.
5	ATOM, BETA	The atom specified is out of range of the parameter list.
6	STOBB	A cell parameter A(1), A(2), or A(3) $\leqslant$ 0.
7	EIGVAL	The eigenvalues are complex.
8	EIGVEC	Only null eigenvectors are found.
9	COSVV	One of the vectors is null.
10	FUNXI	The vector used to specify the direction is null.
11	FUNI	The function specified is out of range. The program requires $0 < XMODF(IN(1),100) \leqslant 15$.

SPECIFICATIONS FOR SUBROUTINES TO COMPUTE NEW TYPES OF FUNCTIONS

To program a new type of function the user selects a function designation integer, i. Function designations 1-15 have already been assigned in the program as written so that normally new designations would be 16, 17....

Subprograms HEDI, PREI, FUNI, and OUTI must each be modified as follows:

1. Change the second IF statement to permit the new function designation.
2. Add a branch to the computed GO TO.
3. Add a CALL statement for the new routine followed by a GO TO 160.

The user then writes four Fortran II subroutines named HEDi, PREi, FUNi, and OUTi as described below. All these subprograms are compiled and added to the binary deck removing the original routines where necessary.

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

HEDi

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

1. The subroutine has no arguments.
2. No COMMON or DIMENSION statements are needed.
3. Put out the heading on tape 9.
4. The first Hollerith character should be zero to cause double spacing.
5. More than one line may be put out if desired.

PREi

This subroutine need be included only if standard errors are to be computed. Its purpose is to instruct the program as

to which parameters are involved in the function to be computed. The program thus avoids computing unnecessary derivatives.

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout the program.
3. Enter the subroutines SETKX and/or SETKB once for each atom involved in the function. See the section "Arithmetic Subprograms Available" for details of these routines.

FUNi

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

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout the program.
3. The significance of the instruction integers IN(K) except for IN(1) is at the discretion of the programmer.
4. The necessary atomic coordinates or temperature factor coefficients are called for by means of subroutines ATOM or BETA.
5. If the metric tensors AA or BB are to be used, the subroutines STOAA and/or STOBB must be entered. See the section "Arithmetic Subprograms Available" for a description of these routines.

6. Store the function at FX in COMMON and RETURN.

OUTi

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

1. The subroutine has no arguments.
2. Include the standard COMMON and DIMENSION statements used throughout Segment 2.
3. The description which probably includes the relevant instruction integers, IN, should be put out on tape 9.
4. The first character of the first line of this description should be a Hollerith zero to cause double spacing.
5. More than one line may be put out if desired.

ARITHMETIC SUBPROGRAMS AVAILABLE

1. CALL SETKX (IN(K))

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

2. CALL SETKB (IN(K))

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

3. CALL STOAA

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

4. CALL STOBB

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

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

DIMENSION Z(3)

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

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

DIMENSION Z(3,3)

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

7. CALL MM (X, Y, Z)

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

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

8. CALL MV (X, Y, Z)

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

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

9. CALL VM (X, Y, Z)

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

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

10. Function VV(X, Y)

DIMENSION X(3), Y(3)

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

11. Function VMV (W, X, Y)

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

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

12. CALL DIFV (X, Y, Z)

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

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

13. CALL SUMV (X, Y, Z)

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

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

14. Function COSVV (X, Y)

DIMENSION X(3), Y(3)

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

15. Function ARCCOS (X)

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

16. CALL NORM (X, Y, Z)

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

Stores at $\underset{\sim}{Z}$ a vector (not a unit vector) perpendicular to both $\underset{\sim}{X}$ and $\underset{\sim}{Y}$. The sense of $\underset{\sim}{Z}$ is that of the vector product $\underset{\sim}{X} \times \underset{\sim}{Y}$. All vectors are referred to the triclinic coordinate system, and it is assumed that the reciprocal metric tensor has been stored at BB in common storage.

17. CALL AXES (U, V, X)

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

Stores three mutually perpendicular vectors (not unit vectors) at X(I,1), X(I,2), and X(I,3). X(I,1) = U(I). X(I,2) is normal to $\underset{\sim}{U}$ and $\underset{\sim}{V}$, i.e., in the direction of $\underset{\sim}{U} \times \underset{\sim}{V}$. X(I,3) is normal to X(I,1) and X(I,2) so as to yield a right-handed coordinate system. All these vectors are referred to the triclinic coordinate system, and it is assumed that the reciprocal metric tensor has been stored at BB in common storage.

18. CALL EIGVAL (W, Y)

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

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

The method used for solving the cubic determinental equation is that described by R. S. Burington, Handbook of Mathematical Tables and Formulas, (Handbook Publishers, Inc., Sandusky, Ohio, 1956), 3rd ed., pp. 7-9.

19. CALL EIGVEC (W, Y, Z)

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

Given an eigenvalue Y of the matrix W, this subroutine stores the corresponding eigenvector Z.

Solving any pair of the three available equations would yield a vector in the desired direction. Because of special symmetry situations, however, the pairs chosen could be redundant so that a null vector would be obtained. The subroutine therefore repeats the calculation with each of the three possible pairs, and the vector of largest magnitude is taken as the correct result. If all three pairs yield null vectors, the subroutine sets an error indicator, because this implies that the direction of the eigenvector is indeterminate.

20. Function TRACE (X)

DIMENSION X(3,3)

Computes the trace of the matrix X.

DISCUSSION OF EXAMPLES

Data for two test problems are included with the card deck for OR FFE. Both are extensions of the hypothetical problem based on alpha quartz which was included with the program OR FLS. Example 1 uses card input only, and tests the present program independently. Example 2 takes part of its input from a tape produced by OR FLS, and tests the two programs together. To obtain the required magnetic tape from OR FLS it is necessary to modify the test data card FLS 1414 by substituting 1 for 0 in column 18.

It should be emphasized again that this problem is a hypothetical one. Although the structure considered is qualitatively that of alpha quartz, the observations used in the OR FLS test are synthetic, and the parameters which result are not related to the true structure of this material.

Silicon atom (2,300) lies on a single twofold rotation axis and has oxygen atoms (1,2), (1,3), (1,300), and (1,305) as four nearest neighbors in an approximately tetrahedral configuration. Example 1 computes the independent distances and angles of this group. The dihedral angle computed is a measure of the distortion of the tetrahedron. The differences computed show how the program can be used to determine whether chemically equivalent but crystallographically distinct distances or angles have significant deviations from each other.

Example 2 includes computations relating to the anisotropic temperature factor coefficients. First the root-mean-square displacements in the principal axis directions are obtained. Then the angles which principal axes of the O atom (1,2) make with the Si-O bond (2,300) (1,2) are computed. Next a cartesian coordinate system is defined in terms of the Si-O vectors (2,300) (1,2) and (2,300) (1,3) so that the principal axes of O can be related to this. Note that the axis with I = 1 is just the Si-O bond direction used above so that the angles with I = 1 repeat those computed earlier.

Because the Si atom is located on a twofold axis, one of its principal axes is constrained to lie in that direction.

By choosing a coordinate system based on Si atoms in different cells, cartesian axis 1 is made to fall on the twofold axis, axis 2 lies in the x,y plane and axis 3 is parallel to z. Principal axes 1 and 3 are both seen to make angles of 90^{o} with cartesian axis 1, as expected. Principal axis 2 should therefore make angles of 0^{o} (or 180^{o}), 90^{o}, and 90^{o} with cartesian axes 1, 2, and 3, respectively. Unfortunately, the results are only approximately correct in the present test problem. The parameters from the hypothetical OR FLS test problem represent atoms which are nearly isotropic, and it is believed that this situation permits round-off errors to cause the observed discrepancies.

Finally three other types of functions are computed to complete the test.

CARD DECKS PROVIDED†

Subprogram	Symbolic card numbers	Column binary card numbers*
Calling program	1 - 246	2051 - 2103**
SUB8	247 - 300	2104 - 2109
SUB10	301 - 321	2110 - 2112
SUB11	322 - 347	2113 - 2115
SUB13	348 - 491	2116 - 2133
SUB19	492 - 508	2134 - 2136
SUB21	509 - 581	2137 - 2145
HEDI	582 - 637	2146 - 2155

Subprogram	Symbolic card numbers	Column binary card numbers*
PREI	638 - 678	2156 - 2162
FUNI	679 - 746	2163 - 2172
OUTI	747 - 786	2173 - 2179
SETKX	787 - 803	2180 - 2182
SETKB	804 - 820	2183 - 2186
STOAA	821 - 840	2187 - 2190
STOBB	841 - 874	2191 - 2197
ATOM	875 - 927	2198 - 2209
BETA	928 - 987	2210 - 2224
MM	988 - 999	2225 - 2228
MV	1000 - 1010	2229 - 2232
VM	1011 - 1021	2233 - 2236
VV	1022 - 1031	2237 - 2239
VMV	1032 - 1040	2240 - 2242
DIFV	1041 - 1049	2243 - 2245
SUMV	1050 - 1058	2246 - 2248
COSVV	1059 - 1075	2249 - 2253
ARCCOS	1076 - 1081	2254 - 2256
NORM	1082 - 1101	2257 - 2260
AXES	1102 - 1113	2261 - 2265
EIGVAL	1114 - 1160	2266 - 2277
EIGVEC	1161 - 1195	2278 - 2284
TRACE	1196 - 1204	2285 - 2287
FUNA	1205 - 1224	2288 - 2292

Subprogram	Symbolic card numbers	Column binary card numbers*
FUND	1225 - 1241	2293 - 2296
HED1	1242 - 1248	2297 - 2299
PRE1	1249 - 1261	2300 - 2302
FUN1	1262 - 1273	2303 - 2305
OUT1	1274 - 1286	2306 - 2308
HED2	1287 - 1293	2309 - 2311
PRE2	1294 - 1306	2312 - 2314
FUN2	1307 - 1318	2315 - 2317
OUT2	1319 - 1331	2318 - 2320
HED3	1332 - 1339	2321 - 2323
PRE3	1340 - 1352	2324 - 2326
FUN3	1353 - 1377	2327 - 2333
OUT3	1378 - 1391	2334 - 2337
HED4	1392 - 1398	2338 - 2340
PRE4	1399 - 1411	2341 - 2343
FUN4	1412 - 1423	2344 - 2346
OUT4	1424 - 1437	2347 - 2350
HED5	1438 - 1444	2351 - 2353
FUN5	1445 - 1456	2354 - 2356
HED6	1457 - 1463	2357 - 2359
PRE6	1464 - 1477	2360 - 2362
FUN6	1478 - 1492	2363 - 2365
OUT6	1493 - 1507	2366 - 2369
FUNB	1508 - 1527	2370 - 2374

Subprogram	Symbolic card numbers	Column binary card numbers*
FUNC	1528 - 1548	2375 - 2379
FUNX	1549 - 1573	2380 - 2386
HED7	1574 - 1581	2387 - 2390
PRE7	1582 - 1593	2391 - 2393
FUN7	1594 - 1606	2394 - 2396
OUT7	1607 - 1619	2397 - 2399
HED8	1620 - 1627	2400 - 2403
PRE8	1628 - 1641	2404 - 2406
FUN8	1642 - 1654	2407 - 2409
OUT8	1655 - 1668	2410 - 2413
HED9	1669 - 1677	2414 - 2417
FUN9	1678 - 1690	2418 - 2420
HED10	1691 - 1699	2421 - 2424
PRE10	1700 - 1713	2425 - 2427
FUN10	1714 - 1726	2428 - 2430
OUT10	1727 - 1741	2431 - 2434
HED11	1742 - 1751	2435 - 2438
FUN11	1752 - 1764	2439 - 2441
FUNR	1765 - 1780	2442 - 2445
FUNCR	1781 - 1799	2446 - 2451
FUNXI	1800 - 1824	2452 - 2457
HED12	1825 - 1833	2458 - 2461
PRE12	1834 - 1847	2462 - 2464
FUN12	1848 - 1860	2465 - 2467

Subprogram	Symbolic card numbers	Column binary card numbers*
OUT12	1861 - 1874	2468 - 2471
HED13	1875 - 1881	2472 - 2474
FUN13	1882 - 1894	2475 - 2477
OUT13	1895 - 1907	2478 - 2480
HED14	1908 - 1915	2481 - 2483
PRE14	1916 - 1929	2484 - 2486
FUN14	1930 - 1943	2487 - 2489
HED15	1944 - 1951	2490 - 2492
FUN15	1952 - 1965	2493 - 2495
ASIN		2496 - 2499***
SETA (Dummy)	1966 - 1970	2500 - 2501
SETP (Dummy)	1971 - 1975	2502 - 2503
SETA (Examples 1 and 2)	1976 - 1982	2504 - 2506
SETP (Example 1)	1983 - 1989	2507 - 2509
SETP (Example 2)	1990 - 1998	2510 - 2512
Transfer card and data for Example 1	1999 - 2022	
Transfer card and data for Example 2	2023 - 2050	

*The column binary cards provided were compiled on an IBM 7090. Most of the subprograms must be recompiled if they are to be used on an IBM 704.

**Card No. 2051 is a control card for the Oak Ridge monitor system. It may not be appropriate at other installations.

***The ASIN routine is included because it is not available from the Oak Ridge library tape. It may not be needed at other installations. Library routines SQRT, COS, and EXIT (which terminates the job) should also be inserted here if they are not supplied by the monitor system.

†Users who received a temporary card deck during 1963 will probably find that the only change has been to add identifying numbers to the final version. The most recent modifications to the program were made in the cards now numbered FFE 072, 073, 162, 939, 940, and 1140-1143. If these cards are verified and corrected where necessary, then the temporary deck will conform to this report.

GLOSSARY OF SYMBOLS

The following list defines the symbols used in the main parts of the program. Some of the independent arithmetic subroutines repeat certain symbols with different meanings, and these are not included in this glossary.

Arrays are represented by symbols followed by their minimum allowable dimensions. All other symbols refer to single-storage variables. Those marked with an asterisk (*) are sometimes read as input data.

*A(6)	Direct cell parameters a, b, c, cos α, cos β, and cos γ.
AA(3,3)	Metric tensor $\underset{\sim}{g}$ where $g_{ij} = \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j$.
AM(21)	Upper triangular part of the variance-covariance matrix associated with the six cell parameters. AM(1) = U_{11}, AM(2) = U_{12},..., AM(6) = U_{16}, AM(7) = U_{22},...., etc.
BB(3,3)	Reciprocal metric tensor $\underset{\sim}{g}^{-1}$ where $(g^{-1})_{ij} = \underset{\sim}{b}_i \cdot \underset{\sim}{b}_j$.
C	Factor C_{ij} used in computing variances in SUB13. $C_{ij} = 1$ if i = j; otherwise $C_{ij} = 2$.
DA(6)	Increments $\Delta a_i = (0.01)\ U_{ii}^{1/2}$.
DFDA(6)	Derivatives $\partial f/\partial a_i$.
DFDP(NV)	Derivatives $\partial f/\partial p_i$.
DMAX	Maximum distance which will be printed when using instructions 101 or 201.
DP(NV)	Increments $\Delta p_i = (0.01)\ V_{ii}^{1/2}$.
E	Standard error, e, of the function including contributions from cell parameter errors and atomic parameter errors.

E1	Standard error, e', of the function including only contributions from least-squares parameter errors.
F	Computed value of function f to be put out.
FX	Computed value of function f as stored by the subroutines FUNi.
*IAM	Cell parameter error indicator. If IAM = 0, cell parameter errors are not to be used. If IAM = 1, they are to be read as standard errors. If IAM = 2, they are to be read as a variance-covariance matrix.
IH	Hundreds digit of the instruction number, IN(1).
*IN(231)	Array of integers used to define the function to be computed. IN(1) specifies the kind of function.
INSAVE	IN(1) saved from the previous instruction integers. The function heading is put out if IN(1) ≠ INSAVE.
*IPM	Atomic parameter error indicator. If IPM = 0, these errors will not be used in computing the standard error of the function. If IPM = 1, they will be used.
*IS(2,3,NS)	Integers representing the non-translational part of the symmetry information. For example, if the Jth symmetry transformation is y-x, -x, 1/3 + z, this information would be stored as follows: TS(1,J) = 0.0 IS(1,1,J) = 2 (for y) IS(2,1,J) = -1 (for -x) TS(2,J) = 0.0 IS(1,2,J) = -1 (for -x) IS(2,2,J) = 0 TS(3,J) = 0.333333 IS(1,3,J) = 3 (for z) IS(2,3,J) = 0
ITF	Temperature factor indicator. ITF = 0 if parameters were read from cards. Otherwise ITF is read from the private output tape of OR FLS and is 1 or 2 for isotropic or anisotropic temperature factors, respectively.

*JB	Position of the first temperature factor coefficient in the parameter list.
*JBP	Period of the temperature factor coefficients in the parameter list.
*JX	Position of the first x-coordinate in the parameter list.
*JXP	Period of the coordinates in the parameter list.
*KI1(NP)	Parameter selection integers. KI1(I) = 1 if P(I) corresponds to a row-column of the variance-covariance matrix, PM. Otherwise KI1(I) = 0.
KI2(NP)	Integers set by subroutine PREi to specify the parameters involved in the function being computed. KI2(I) is set to 1 if P(I) is involved in the function. Otherwise KI2(I) = 0.
KK	Index used so that PM(KK) is a diagonal element of the variance-covariance matrix.
KKD	Increment to be added to KK to step from one diagonal element of PM to the next.
LNZ	Integer saved to record that DFDP(LNZ) is the last non-zero derivative in the array.
NA	Number of atoms in the parameter list as specified by the instruction integers for certain multivalued functions.
NG	Error indicator set to a non-zero integer when an error is found in the course of calculating a function or its derivative. See the section "Error Indicators" for a list of these errors.
NM	NV(NV+1)/2, the number of elements in the upper triangular part of the variance-covariance matrix, PM.
*NP	Number of parameters in the parameter list.
NQ	Number of scale factors in a parameter list which has been read from the private output tape of OR FLS.

*NS	Number of symmetry cards read.
NSP	NS+1, the number of symmetry positions including the basic asymmetric unit.
*NV	Order of the variance-covariance matrix for the atomic parameters.
*P(NP)	List of atomic parameters read either from cards or from the private output tape of OR FLS.
*PM(NM)	Upper triangular part of variance-covariance matrix associated with the atomic parameters PM(1) = V_{11}, PM(2) = V_{12}, ..., PM(NV) = $V_{1,NV}$, PM(NV+1) = V_{22}, ..., etc.
ROW(6)	Auxiliary array used in putting out the matrix AM.
SAVEA	Temporary storage for a cell parameter which is being incremented during the derivative calculation.
SAVEP	Temporary storage for an atomic parameter which is being incremented during the derivative calculation.
*SCALE	Constant used to scale the variance-covariance matrix if it is read from cards.
*TITLE(12)	Alphanumeric title read at the start of the problem and transcribed to the output.
*TS(3,NS)	Translational part of symmetry information. (See IS for an example.)
VARA	Variance of f based on the cell parameter errors only.
VARP	Variance of f based on the atomic parameter errors only.

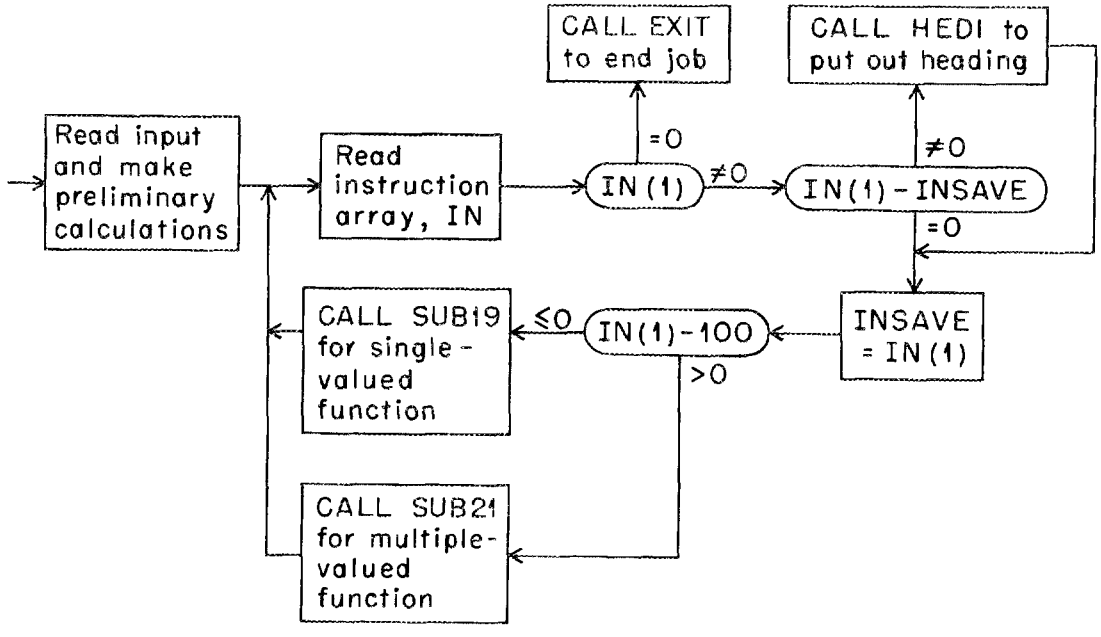

Figure 1. Schematic flow diagram of the main program showing the subprograms called by it.

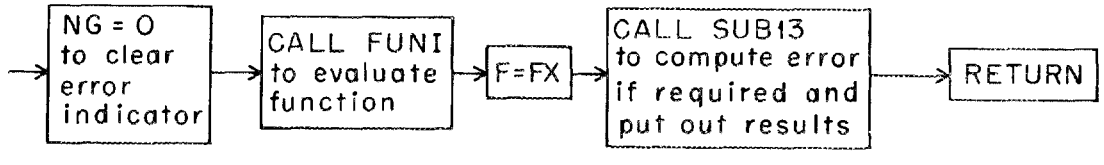

Figure 2. SUB19 which controls the calculation and output for a single-valued function.

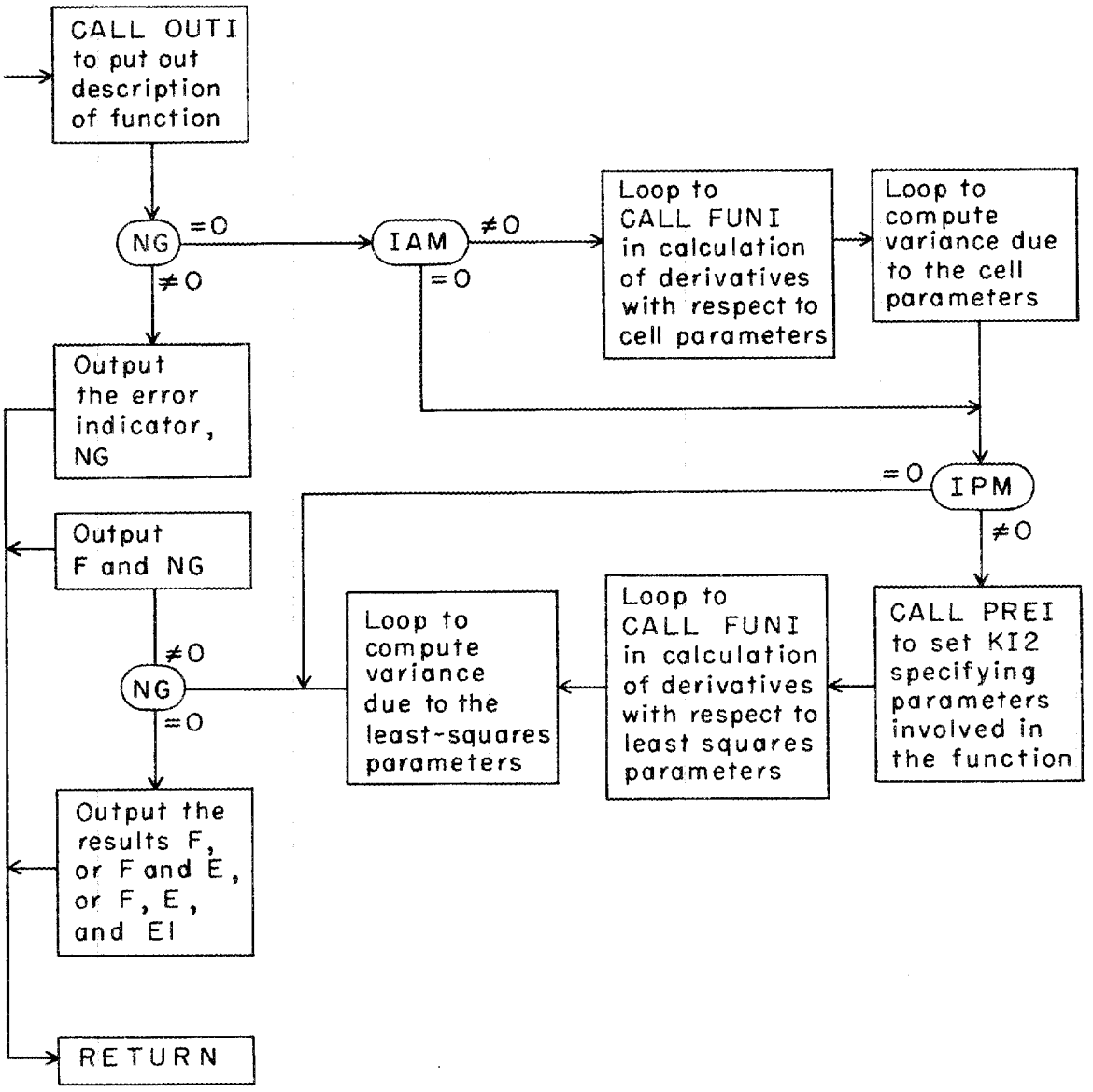

Figure 3. SUB13 which calculates the error if required and puts out the results.

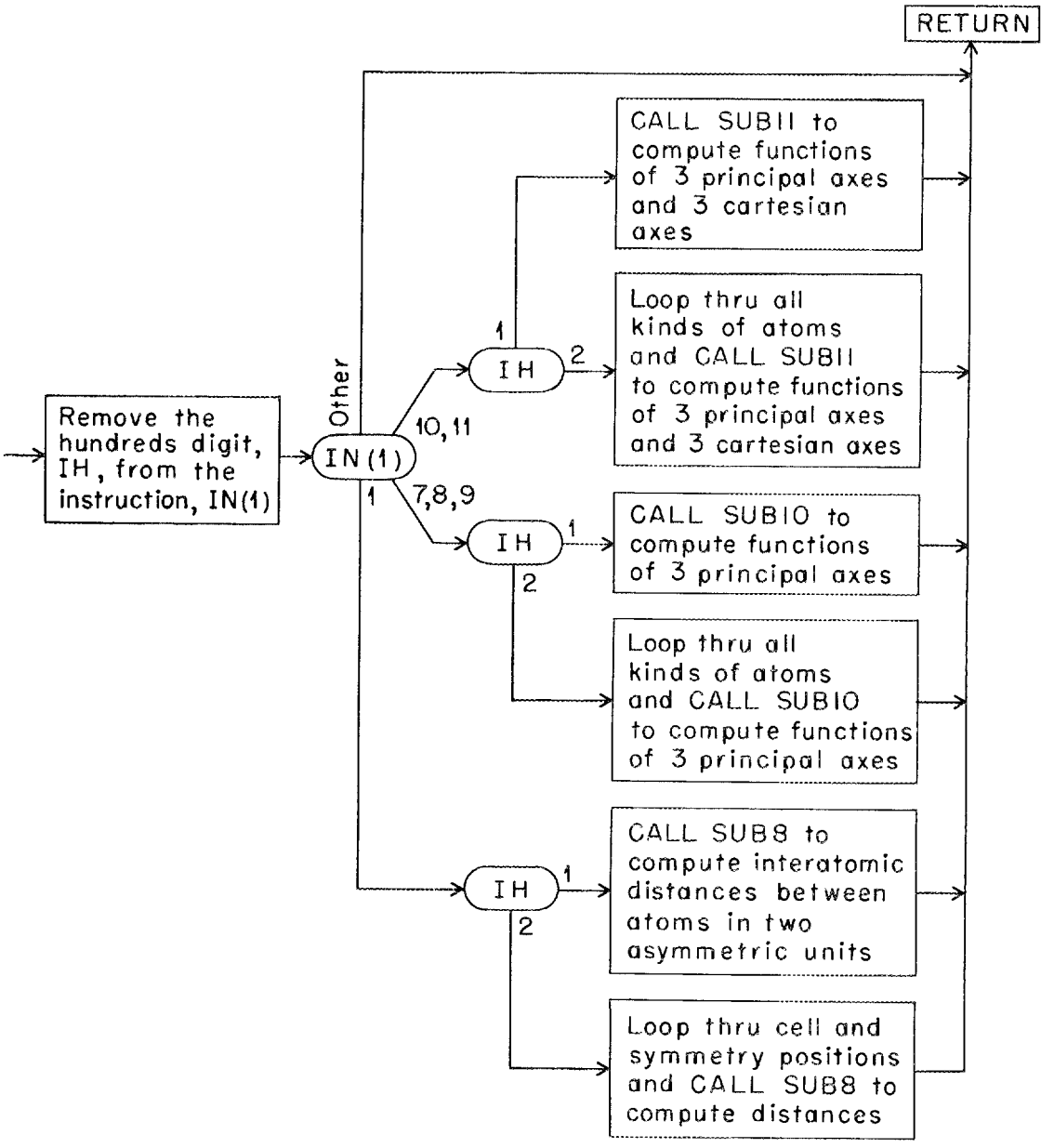

Figure 4. SUB21 which controls the calculations for multiple-values functions.

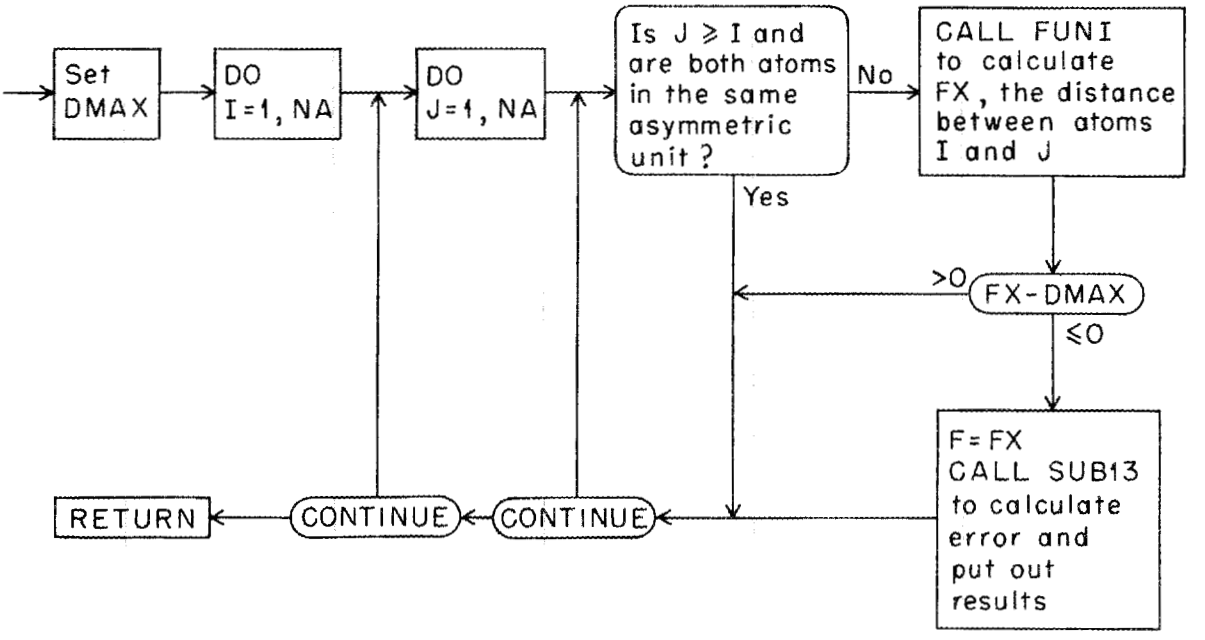

Figure 5. SUB8 which calculates all distances less than DMAX between atoms of two asymmetric units.

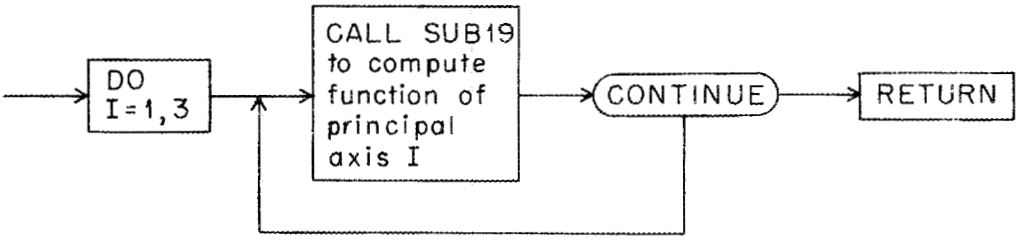

Figure 6. SUB10 which controls the calculation of funtions of each of the three principal axes of thermal motion.

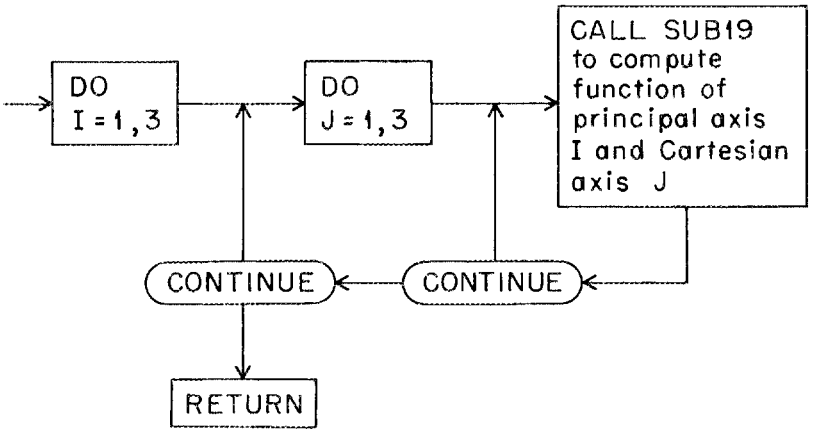

Figure 7. SUB11 which controls the calculation of functions of each of the three principal axes and of three axes of a specified cartesian coordinate system.

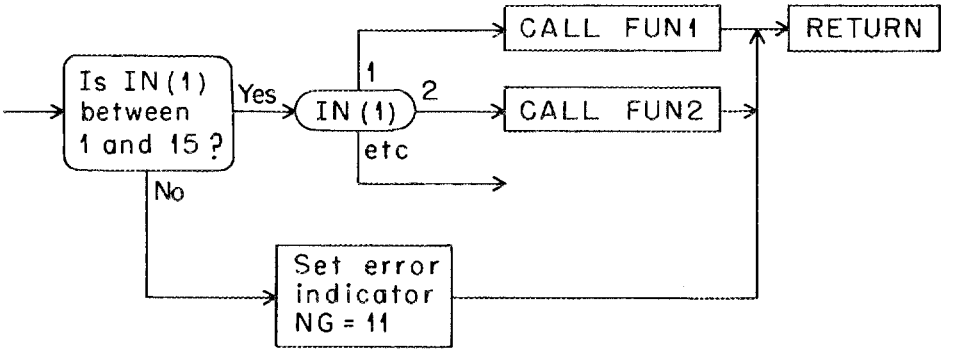

Figure 8. FUNI which transfers control to the appropriate function-calculating subroutine. HEDI, PREI, and OUTI are almost analogous to FUNI.

SYMBOLIC PROGRAM LISTING

```
*TYPE(FORTRAN)                                                          FFE  001
C       OR FFE. FORTRAN CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM     FFE  002
C       CALLING PROGRAM                                                 FFE  003
                                                                        FFE  004
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE FFE  005
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP FFE  006
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  007
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)    FFE  008
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  009
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)                       FFE  010
                                                                        FFE  011
C       READ AND PUT OUT TITLE AND CONTROL CARD                         FFE  012
        READ INPUT TAPE 10,00102,(TITLE(I),I#1,12)                      FFE  013
00102 FORMAT (12A6)                                                     FFE  014
        WRITE OUTPUT TAPE 9,00104,(TITLE(I),I#1,12)                     FFE  015
00104 FORMAT (1H1,12A6)                                                 FFE  016
        READ INPUT TAPE 10,00202,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB         FFE  017
00202 FORMAT (24I3)                                                     FFE  018
        IF(NP)00297,00294,00297                                         FFE  019
                                                                        FFE  020
00294     WRITE OUTPUT TAPE 9,00295                                     FFE  021
00295     FORMAT (39H0INPUT DATA TO BE READ FROM OR FLS TAPE)           FFE  022
          GO TO 00301                                                   FFE  023
                                                                        FFE  024
00297     WRITE OUTPUT TAPE 9,00298,NP                                  FFE  025
00298     FORMAT (33H0INPUT DATA TO BE READ FROM CARDS/                 FFE  026
     1       34H0NUMBER OF STRUCTURE PARAMETERS ISI4)                   FFE  027
                                                                        FFE  028
00301 WRITE OUTPUT TAPE 9,00302                                         FFE  029
00302 FORMAT (68H0VARIANCE-COVARIANCE MATRIX AND PARAMETER SELECTION INFFFE  030
     1ORMATION WILL)                                                    FFE  031
        IF(IPM)00308,00305,00308                                        FFE  032
                                                                        FFE  033
00305     WRITE OUTPUT TAPE 9,00306                                     FFE  034
00306     FORMAT (12H NOT BE USED)                                      FFE  035
          GO TO 00310                                                   FFE  036
                                                                        FFE  037
00308     WRITE OUTPUT TAPE 9,00309                                     FFE  038
00309     FORMAT (8H BE USED)                                           FFE  039
                                                                        FFE  040
00310 WRITE OUTPUT TAPE 9,00311,NS                                      FFE  041
00311 FORMAT (28H0NUMBER OF SYMMETRY CARDS ISI3)                        FFE  042
        WRITE OUTPUT TAPE 9,00314                                       FFE  043
00314 FORMAT (26H0CELL PARAMETER ERRORS ARE)                            FFE  044
        IF(IAM-1)00316,00319,00322                                      FFE  045
                                                                        FFE  046
00316     WRITE OUTPUT TAPE 9,00317                                     FFE  047
00317     FORMAT (15H NOT TO BE USED)                                   FFE  048
          GO TO 00401                                                   FFE  049
                                                                        FFE  050
00319     WRITE OUTPUT TAPE 9,00320                                     FFE  051
00320     FORMAT (42H TO BE READ IN THE FORM OF STANDARD ERRORS)        FFE  052
          GO TO 00401                                                   FFE  053
                                                                        FFE  054
00322     WRITE OUTPUT TAPE 9,00323                                     FFE  055
00323     FORMAT (48H TO BE READ IN THE FORM OF A VARIANCE-COVARIANCE   FFE  056
     1       7H MATRIX)                                                 FFE  057
                                                                        FFE  058
00401 IF(NP)01001,01001,00501                                           FFE  059
                                                                        FFE  060
C         READ PARAMETERS AND VARIANCE-COVARIANCE MATRIX FROM CARDS     FFE  061
00501     WRITE OUTPUT TAPE 9,00502,NV                                  FFE  062
00502     FORMAT (44H0ORDER OF THE VARIANCE-COVARIANCE MATRIX FOR       FFE  063
     1       28H THE STRUCTURE PARAMETERS ISI3)                         FFE  064
          IF(JXP)00509,00509,00505                                      FFE  065
                                                                        FFE  066
```

```
00505       WRITE OUTPUT TAPE 9,00506,JXP,JX                                  FFE  067
00506       FORMAT (41HOPERIOD OF THE POSITION PARAMETERS IN THE              FFE  068
     1         18H PARAMETER LIST ISI3/22HOPOSITION OF THE FIRST               FFE  069
     2         38H X COORDINATE IN THE PARAMETER LIST ISI3)                    FFE  070
                                                                               FFE  071
00509    ITF#0                                                                FFE  072
         IF(JBP)00601,00601,00510                                             FFE  073
                                                                               FFE  074
00510       WRITE OUTPUT TAPE 9,00511,JBP,JB                                  FFE  075
00511       FORMAT (46HOPERIOD OF THE TEMPERATURE FACTOR COEFFICIENTS         FFE  076
     1         25H IN THE PARAMETER LIST ISI3/16HOPOSITION OF THE              FFE  077
     2         44H FIRST TEMPERATURE FACTOR COEFFICIENT IN THE                 FFE  078
     3         18H PARAMETER LIST ISI3)                                        FFE  079
                                                                               FFE  080
00601    READ INPUT TAPE 10,00603,(P(I),I#1,NP)                               FFE  081
00603    FORMAT (8E9.4)                                                       FFE  082
         IF(IPM)00801,02101,00801                                             FFE  083
                                                                               FFE  084
00801       READ INPUT TAPE 10,00802,(KII(I),I#1,NP)                          FFE  085
00802       FORMAT (72I1)                                                     FFE  086
            NM#(NV*(NV+1))/2                                                  FFE  087
            READ INPUT TAPE 10,00905,SCALE                                    FFE  088
            READ INPUT TAPE 10,00905,(PM(I),I#1,NM)                           FFE  089
00905       FORMAT (6E12.6)                                                   FFE  090
            DO 00952 I#1,NM                                                   FFE  091
                                                                              FFE  092
00952          PM(I)#PM(I)*SCALE                                              FFE  093
                                                                              FFE  094
            GO TO 02101                                                       FFE  095
                                                                              FFE  096
C        READ PARAMETERS AND VARIANCE-COVARIANCE MATRIX                       FFE  097
C                                              FROM OR FLS TAPE               FFE  098
01001    REWIND 3                                                             FFE  099
         READ INPUT TAPE 3,00202,ITF,NQ,NP                                    FFE  100
         WRITE OUTPUT TAPE 9,01004,NP                                         FFE  101
01004    FORMAT (34HONUMBER OF STRUCTURE PARAMETERS ISI4)                      FFE  102
         READ INPUT TAPE 3,01007,(P(I),I#1,NP)                                FFE  103
01007    FORMAT (10E12.8)                                                     FFE  104
         JX#NQ+4                                                              FFE  105
         JB#NQ+7                                                              FFE  106
         IF(ITF-1)01301,01301,01401                                           FFE  107
                                                                              FFE  108
01301       JXP#6                                                             FFE  109
            JBP#6                                                             FFE  110
            GO TO 01501                                                       FFE  111
                                                                              FFE  112
01401       JXP#11                                                            FFE  113
            JBP#11                                                            FFE  114
                                                                              FFE  115
01501    WRITE OUTPUT TAPE 9,00506,JXP,JX                                     FFE  116
         WRITE OUTPUT TAPE 9,00511,JBP,JB                                     FFE  117
         IF(IPM)01701,02101,01701                                             FFE  118
                                                                              FFE  119
01701       READ INPUT TAPE 3,00802,(KII(I),I#1,NP)                           FFE  120
            READ INPUT TAPE 3,00202,NV                                        FFE  121
            WRITE OUTPUT TAPE 9,00502,NV                                      FFE  122
            NM#(NV*(NV+1))/2                                                  FFE  123
            READ INPUT TAPE 3,02002,(PM(K),K#1,NM)                            FFE  124
02002       FORMAT (8E15.8)                                                   FFE  125
                                                                              FFE  126
C     PUT OUT INPUT PARAMETERS                                                FFE  127
02101 WRITE OUTPUT TAPE 9,02102                                               FFE  128
02102 FORMAT (1H1HOINPUT DATA/2IHO  I     P(I)  KII(I)/IH )                   FFE  129
      DO 02104 I#1,NP                                                         FFE  130
                                                                              FFE  131
02104    WRITE OUTPUT TAPE 9,02105,I,P(I),KII(I)                              FFE  132
02105    FORMAT (1H I3,F10.4,I4)                                              FFE  133
                                                                              FFE  134
C     READ AND PUT OUT CELL PARAMETERS                                        FFE  135
      READ INPUT TAPE 10,02202,(A(I),I#1,6)                                   FFE  136
```

```
02202 FORMAT (6F9.4)                                                    FFE  137
      WRITE OUTPUT TAPE 9,00104,(TITLE(I),I#1,12)                       FFE  138
      WRITE OUTPUT TAPE 9,02205,(A(I),I#1,6)                            FFE  139
02205 FORMAT(16HOCELL PARAMETERS/1H06F11.4)                             FFE  140
      IF(IAM-1)03401,02401,02701                                        FFE  141
                                                                        FFE  142
C        READ STANDARD ERRORS OF CELL PARAMETERS                        FFE  143
02401    DO 02402 I#1,21                                                FFE  144
                                                                        FFE  145
02402       AM(I)#0.0                                                   FFE  146
                                                                        FFE  147
         READ INPUT TAPE 10,02202,AM(1),AM(7),AM(12),AM(16),            FFE  148
     1                                          AM(19),AM(21)          FFE  149
         WRITE OUTPUT TAPE 9,02503,AM(1),AM(7),AM(12),AM(16),           FFE  150
     1                                          AM(19),AM(21)          FFE  151
02503    FORMAT (49HOSTANDARD ERRORS, RESPECTIVELY, OF THE ABOVE CELL   FFE  152
     1      11H PARAMETERS/1H06F11.4)                                   FFE  153
         DO 02602 I#1,21                                                FFE  154
                                                                        FFE  155
02602       AM(I)#AM(I)*AM(I)                                           FFE  156
                                                                        FFE  157
         GO TO 03201                                                    FFE  158
                                                                        FFE  159
C        READ VARIANCE-COVARIANCE MATRIX FOR CELL PARAMETERS            FFE  160
02701    READ INPUT TAPE 10,00603,(AM(I),I#1,21)                        FFE  161
         WRITE OUTPUT TAPE 9,2703                                       FFE  162
02703    FORMAT (47HOVARIANCE-COVARIANCE MATRIX FOR CELL PARAMETERS)     FFE  163
         IJ#1                                                           FFE  164
         DO 03101 I#1,6                                                 FFE  165
                                                                        FFE  166
            DO 02902 J#1,6                                              FFE  167
                                                                        FFE  168
02902          ROW(J)#0.0                                               FFE  169
                                                                        FFE  170
            DO 03003 J#1,6                                              FFE  171
                                                                        FFE  172
               ROW(J)#AM(IJ)                                            FFE  173
03003          IJ#IJ+1                                                  FFE  174
                                                                        FFE  175
03101       WRITE OUTPUT TAPE 9,03102,(ROW(J),J#1,6)                    FFE  176
03102       FORMAT (1H06F11.4)                                          FFE  177
                                                                        FFE  178
C        COMPUTE CELL PARAMETER INCREMENTS USED TO OBTAIN DERIVATIVES   FFE  179
03201    K#1                                                            FFE  180
         L#6                                                            FFE  181
         DO 03303 I#1,6                                                 FFE  182
                                                                        FFE  183
            DA(I)#(0.01)*SQRTF(AM(K))                                   FFE  184
            K#K+L                                                       FFE  185
03303       L#L-1                                                       FFE  186
                                                                        FFE  187
03401 IF(NS)03701,03701,03601                                           FFE  188
                                                                        FFE  189
C        READ AND PUT OUT SYMMETRY TRANSFORMATIONS                      FFE  190
03601    READ INPUT TAPE 10,03602,(((TS(I,J),(IS(K,I,J),K#1,2),I#1,3),  FFE  191
     1                                                  J#1,NS)         FFE  192
03602    FORMAT (F11.6,2I2,F11.6,2I2,F11.6,2I2)                         FFE  193
         WRITE OUTPUT TAPE 9,03604                                      FFE  194
03604    FORMAT (21HOSYMMETRY INFORMATION/19HO      TRANSFORMED X       FFE  195
     1      48H            TRANSFORMED Y            TRANSFORMED Z/1H )  FFE  196
         WRITE OUTPUT TAPE 9,03608,(((TS(I,J),(IS(K,I,J),K#1,2),I#1,3), FFE  197
     1                                                  J#1,NS)         FFE  198
03608    FORMAT (1H F13.6,2I2,F20.6,2I2,F20.6,2I2)                      FFE  199
                                                                        FFE  200
03701 IF(IPM)03801,04001,03801                                          FFE  201
                                                                        FFE  202
C        COMPUTE PARAMETER INCREMENTS USED TO OBTAIN DERIVATIVES        FFE  203
03801    K#1                                                            FFE  204
         L#NV                                                           FFE  205
         DO 03903 I#1,NV                                                FFE  206
```

```
                                                                        FFE  207
            DP(I)#(0.01)*SQRTF(PM(K))                                   FFE  208
            K#K+L                                                       FFE  209
03903       L#L-1                                                       FFE  210
                                                                        FFE  211
04001 WRITE OUTPUT TAPE 9,04002,(TITLE(I),I#1,12)                       FFE  212
04002 FORMAT (1H1,12A6/1H )                                             FFE  213
                                                                        FFE  214
C       READ ONE SET OF INSTRUCTIONS                                    FFE  215
04101   K#1                                                             FFE  216
        DO 04501 I#1,10                                                 FFE  217
                                                                        FFE  218
            L#K+23                                                      FFE  219
            READ INPUT TAPE 10,00202,(IN(J),J#K,L)                      FFE  220
            IF(IN(L))04501,04601,04501                                  FFE  221
                                                                        FFE  222
04501       K#L                                                         FFE  223
                                                                        FFE  224
04601   IF(IN(1))04801,04701,04801                                      FFE  225
                                                                        FFE  226
C           END OF JOB                                                  FFE  227
04701       CALL EXIT                                                   FFE  228
                                                                        FFE  229
04801   IF(IN(1)-INSAVE)04901,05001,04901                               FFE  230
                                                                        FFE  231
C           PUT OUT HEADING FOR NEW TYPE OF FUNCTION                    FFE  232
04901       CALL HED1(IN(1))                                            FFE  233
                                                                        FFE  234
05001   INSAVE#IN(1)                                                    FFE  235
        IF(IN(1)-100)05101,05101,05201                                  FFE  236
                                                                        FFE  237
C           COMPUTE SINGLE-VALUED FUNCTION                              FFE  238
05101       CALL SUB19                                                  FFE  239
            GO TO 04101                                                 FFE  240
                                                                        FFE  241
C           COMPUTE MULTIPLE-VALUED FUNCTION                            FFE  242
05201       CALL SUB21                                                  FFE  243
            GO TO 04101                                                 FFE  244
                                                                        FFE  245
      END(0,1,0,0,0)                                                    FFE  246
*TYPE(FORTRAN)                                                          FFE  247
C     COMPUTE ALL DISTANCES BETWEEN TWO ASYMMETRIC UNITS                FFE  248
      SUBROUTINE SUB8                                                   FFE  249
                                                                        FFE  250
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  251
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  252
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  253
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  254
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  255
      DIMENSION P(300),ROW(6),KI1(300),KI2(200)                         FFE  256
                                                                        FFE  257
C     SET MAXIMUM DISTANCE ACCEPTED                                     FFE  258
      IF(IN(6))107,107,111                                              FFE  259
                                                                        FFE  260
  107   DMAX#4.0                                                        FFE  261
        GOTO113                                                         FFE  262
                                                                        FFE  263
  111   DMAX#FLOATF(IN(6))/10.0                                         FFE  264
                                                                        FFE  265
  113 NA#IN(2)                                                          FFE  266
      IF(NA)217,217,117                                                 FFE  267
                                                                        FFE  268
C     START LOOP FOR FIRST ATOM                                         FFE  269
  117 DO215I#1,NA                                                       FFE  270
                                                                        FFE  271
        IN(2)#I                                                         FFE  272
                                                                        FFE  273
C       START LOOP FOR SECOND ATOM                                      FFE  274
        DO213J#1,NA                                                     FFE  275
                                                                        FFE  276
```

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C           TEST TO AVOID DUPLICATION                                       FFE  277
            IF(IN(3)-IN(5))201,125,201                                      FFE  278
                                                                            FFE  279
  125          IF(J-I)201,215,215                                           FFE  280
                                                                            FFE  281
  201       IN(4)#J                                                         FFE  282
            NG#0                                                            FFE  283
                                                                            FFE  284
C           COMPUTE AND TEST DISTANCE                                       FFE  285
            CALL FUNI(IN(I))                                                FFE  286
            IF(FX-DMAX)209,209,213                                          FFE  287
                                                                            FFE  288
C              COMPUTE ERROR AND PUT OUT RESULTS                            FFE  289
  209          F#FX                                                         FFE  290
               CALLSUBI3                                                    FFE  291
                                                                            FFF  292
  213       CONTINUE                                                        FFE  293
C           END LOOP FOR SECOND ATOM                                        FFE  294
                                                                            FFE  295
  215    CONTINUE                                                           FFE  296
C        END LOOP FOR FIRST ATOM                                            FFE  297
                                                                            FFE  298
  217 RETURN                                                                FFE  299
      END(0,1,0,0,0)                                                        FFE  300
*TYPE(FORTRAN)                                                             FFE  301
C     MULTIVALUED FUNCTIONS 7, 8, AND 9                                     FFE  302
      SUBROUTINE SUBI0                                                      FFE  303
                                                                            FFE  304
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE       FFE  305
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP      FFE  306
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2     FFE  307
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)          FFE  308
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  309
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                             FFE  310
                                                                            FFE  311
C     START LOOP THRU PRINCIPAL AXES                                        FFE  312
      DO109I#1,3                                                            FFE  313
                                                                            FFE  314
         IN(4)#I                                                            FFE  315
                                                                            FFE  316
C        COMPUTE AND PUT OUT FUNCTION AND ERROR                             FFE  317
  109    CALLSUBI9                                                          FFE  318
                                                                            FFE  319
      RETURN                                                                FFE  320
      END(0,1,0,0,0)                                                        FFE  321
*TYPE(FORTRAN)                                                             FFE  322
C     MULTIVALUED FUNCTIONS 10 AND 11                                       FFE  323
      SUBROUTINE SUBI1                                                      FFE  324
                                                                            FFE  325
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE       FFE  326
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP      FFE  327
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2     FFE  328
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)          FFE  329
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  330
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                             FFE  331
                                                                            FFE  332
C     START LOOP THRU PRINCIPAL AXES                                        FFE  333
      DO113I#1,3                                                            FFE  334
                                                                            FFE  335
         IN(4)#I                                                            FFE  336
                                                                            FFE  337
C        START LOOP THRU REFERENCE AXES                                     FFE  338
         DO113J#1,3                                                         FFE  339
                                                                            FFE  340
            IN(5)#J                                                         FFE  341
                                                                            FFF  342
C           COMPUTE AND PUT OUT FUNCTION AND ERROR                          FFE  343
  113       CALLSUBI9                                                       FFF  344
                                                                            FFE  345
      RETURN                                                                FFE  346
```

```
      END(0,1,0,0,0)                                                    FFE  347
*TYPE(FORTRAN)                                                          FFE  348
C     ERROR CALCULATION AND OUTPUT                                      FFE  349
      SUBROUTINE SUB13                                                  FFE  350
                                                                        FFE  351
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  352
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE  353
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  354
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  355
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  356
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  357
                                                                        FFE  358
C     PUT OUT FUNCTION DESCRIPTION                                      FFE  359
      CALL OUTI(IN(1))                                                  FFE  360
      IF(NG)107,113,107                                                 FFE  361
                                                                        FFE  362
C        PUT OUT ERROR INDICATOR IF NOT ZERO                            FFE  363
  107 WRITE OUTPUT TAPE 9,109,NG                                        FFE  364
  109 FORMAT (1H 5IX,3H***I3)                                           FFE  365
      GO TO 723                                                         FFE  366
                                                                        FFE  367
  113 VARA#0.0                                                          FFE  368
      VARP#0.0                                                          FFE  369
      IF(IAM)119,313,119                                                FFE  370
                                                                        FFE  371
C        COMPUTE DERIVATIVES WITH RESPECT TO CELL PARAMETERS            FFE  372
  119 DO 211 I#1,6                                                      FFE  373
                                                                        FFE  374
          IF(DA(I))201,123,201                                          FFE  375
                                                                        FFE  376
  123        DFDA(I)#0.0                                              FFE  377
             GO TO 211                                                  FFE  378
                                                                        FFE  379
  201        SAVEA#A(I)                                               FFE  380
             A(I)#A(I)+DA(I)                                          FFE  381
             CALL FUNI(IN(1))                                         FFE  382
             A(I)#SAVEA                                               FFE  383
             DFDA(I)#(FX-F)/DA(I)                                     FFE  384
                                                                        FFE  385
  211     CONTINUE                                                      FFE  386
                                                                        FFE  387
C        COMPUTE VARIANCE BASED ON CELL PARAMETERS                      FFE  388
         K#1                                                            FFE  389
         L#6                                                            FFE  390
         DO 311 I#1,6                                                   FFE  391
                                                                        FFE  392
            IF(DFDA(I))225,221,225                                      FFE  393
                                                                        FFE  394
  221          K#K+L                                                   FFE  395
               GO TO 311                                                FFE  396
                                                                        FFE  397
  225          C#1.0                                                   FFE  398
               DO 309 J#I,6                                             FFE  399
                                                                        FFE  400
                  IF(DFDA(J))305,307,305                                FFE  401
                                                                        FFE  402
  305                VARA#VARA+C*DFDA(I)*DFDA(J)*AM(K)                 FFE  403
                                                                        FFE  404
  307              K#K+1                                               FFE  405
  309              C#2.0                                               FFE  406
                                                                        FFE  407
  311     L#L-1                                                         FFE  408
                                                                        FFE  409
  313 IF(IPM)315,615,315                                                FFE  410
                                                                        FFE  411
C        SELECT DERIVATIVES TO BE COMPUTED                              FFE  412
  315 DO 319 I#1,NP                                                     FFE  413
                                                                        FFE  414
  319     KI2(I)#0                                                      FFE  415
                                                                        FFE  416
```

```
      CALL PRFI(IN(I))                                                  FFE  417
                                                                        FFE  418
C     COMPUTE DERIVATIVES WITH RESPECT TO STRUCTURE PARAMETERS          FFE  419
      J#0                                                               FFE  420
      DO 513 I#1,NV                                                     FFE  421
                                                                        FFE  422
403      J#J+1                                                          FFE  423
         IF(KI1(J))407,403,407                                          FFE  424
                                                                        FFE  425
407      IF(KI2(J))413,409,413                                          FFE  426
                                                                        FFE  427
409         DFDP(I)#0.0                                                 FFE  428
            GO TO 513                                                   FFE  429
                                                                        FFE  430
413         IF(DP(I))501,409,501                                        FFE  431
                                                                        FFE  432
501         SAVEP#P(J)                                                  FFE  433
            P(J)#P(J)+DP(I)                                             FFE  434
            CALL FUNI(IN(I))                                            FFE  435
            P(J)#SAVEP                                                  FFE  436
            DFDP(I)#(FX-F)/DP(I)                                        FFE  437
            LNZ#I                                                       FFE  438
                                                                        FFE  439
513      CONTINUE                                                       FFE  440
                                                                        FFE  441
C     COMPUTE VARIANCE BASED ON STRUCTURE PARAMETERS                    FFE  442
      KK#1                                                              FFE  443
      KKD#NV                                                            FFE  444
      DO 613 I#1,LNZ                                                    FFE  445
                                                                        FFE  446
         IF(DFDP(I))523,612,523                                         FFE  447
                                                                        FFE  448
523         K#KK                                                        FFE  449
            C#1.0                                                       FFE  450
            DO 611 J#1,LNZ                                              FFE  451
                                                                        FFE  452
               IF(DFDP(J))607,609,607                                   FFE  453
                                                                        FFE  454
607               VARP#VARP+C*DFDP(I)*DFDP(J)*PM(K)                     FFE  455
                                                                        FFE  456
609            K#K+1                                                    FFE  457
611            C#2.0                                                    FFE  458
                                                                        FFE  459
612      KK#KK+KKD                                                      FFE  460
613      KKD#KKD-1                                                      FFE  461
                                                                        FFE  462
615 IF(NG)617,623,617                                                   FFE  463
                                                                        FFE  464
C        PUT OUT ERROR INDICATOR IF NOT ZERO                            FFE  465
617      WRITE OUTPUT TAPE 9,619,F,NG                                   FFE  466
619      FORMAT (1H 48X,F9.4,6X,3H***I3)                                FFE  467
         GO TO 723                                                      FFE  468
                                                                        FFE  469
C     COMPUTE STANDARD ERRORS AND PUT OUT RESULTS                       FFE  470
623   EI#SQRTF(VARP)                                                    FFE  471
      E#SQRTF(VARP+VARA)                                                FFE  472
      IF(IPM)703,705,703                                                FFE  473
                                                                        FFE  474
703   IF(IAM)707,713,707                                                FFE  475
                                                                        FFE  476
705   IF(IAM)713,719,713                                                FFE  477
                                                                        FFE  478
707      WRITE OUTPUT TAPE 9,709,F,E,EI                                 FFE  479
709      FORMAT (1H 48X,F9.4,5H +OR-F7.4,2H (F7.4,1H))                  FFE  480
         GO TO 723                                                      FFE  481
                                                                        FFE  482
713      WRITE OUTPUT TAPE 9,715,F,E                                    FFE  483
715      FORMAT (1H 48X,F9.4,5H +OR-F7.4)                               FFE  484
         GO TO 723                                                      FFE  485
                                                                        FFE  486
```

```
  719       WRITE OUTPUT TAPE 9,721,F                                    FFE  487
  721       FORMAT (1H 48X,F9.4)                                         FFE  488
                                                                         FFE  489
  723 RETURN                                                             FFE  490
      END(0,1,0,0,0)                                                     FFE  491
*TYPE(FORTRAN)                                                           FFE  492
C     FUNCTION AND ERROR CALCULATION                                     FFE  493
      SUBROUTINE SUB19                                                   FFE  494
                                                                         FFE  495
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE  496
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE  497
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE  498
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE  499
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  500
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE  501
                                                                         FFE  502
      NG#0                                                               FFE  503
      CALL FUNI(IN(1))                                                   FFE  504
      F#FX                                                               FFE  505
      CALLSUB13                                                          FFE  506
      RETURN                                                             FFE  507
      END(0,1,0,0,0)                                                     FFE  508
*TYPE(FORTRAN)                                                           FFE  509
C     COMPUTE MULTIVALUED FUNCTIONS                                      FFE  510
*     SUBROUTINE SUB21                                                   FFE  511
                                                                         FFE  512
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE  513
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE  514
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE  515
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE  516
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  517
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE  518
                                                                         FFE  519
C     UNPACK INSTRUCTION NUMBER                                          FFE  520
      IH#IN(1)/100                                                       FFE  521
      IN(1)#IN(1)-100*IH                                                 FFE  522
                                                                         FFE  523
C     TRANSFER TO APPROPRIATE SECTION                                    FFE  524
      IF(IN(1)-11)111,111,319                                            FFE  525
  111 IF(IN(1)-9)113,113,305                                             FFE  526
  113 IF(IN(1)-6)115,115,215                                             FFE  527
  115 IF(IN(1)-1)117,117,319                                             FFE  528
                                                                         FFE  529
  117    IF(IH-1)119,119,123                                             FFE  530
                                                                         FFE  531
C           COMPUTE ALL DISTANCES BETWEEN TWO UNITS                      FFE  532
  119       CALLSUB8                                                     FFE  533
            GOTO319                                                      FFE  534
                                                                         FFE  535
C           COMPUTE DISTANCES INVOLVING BASIC UNIT AND ALL OTHERS        FFE  536
  123       NA#IN(2)                                                     FFE  537
            NSP#NS+1                                                     FFE  538
            IN(3)#0                                                      FFE  539
            DO211I#1,8                                                   FFE  540
                                                                         FFE  541
               DO211J#1,NSP                                              FFE  542
                                                                         FFE  543
                  IN(2)#NA                                               FFE  544
                  IN(5)#100*(I-1)+J-1                                    FFE  545
  211             CALLSUB8                                               FFE  546
                                                                         FFE  547
            GOTO319                                                      FFE  548
                                                                         FFE  549
  215    IF(IH-1)217,217,221                                             FFE  550
                                                                         FFE  551
C           COMPUTE FUNCTIONS INVOLVING THREE PRINCIPAL AXES             FFE  552
  217       CALLSUB10                                                    FFE  553
            GOTO319                                                      FFE  554
                                                                         FFE  555
C           COMPUTE FUNCTIONS INVOLVING THREE PRINCIPAL AXES             FFE  556
```

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C                                                    FOR ALL ATOMS                  FFE  557
                                                                                    FFE  558
  221       NA#IN(2)                                                                FFE  559
            DO301I#1,NA                                                             FFE  560
                                                                                    FFE  561
               IN(2)#I                                                              FFE  562
  301          CALLSUB10                                                           FFE  563
                                                                                    FFE  564
            GOTO319                                                                 FFE  565
                                                                                    FFE  566
  305    IF(IH-1)307,307,311                                                        FFE  567
C                                                                                   FFE  568
            COMPUTE FOR ALL PRINCIPAL AXES AND ALL REFERENCE AXES                   FFE  569
  307       CALLSUB11                                                             FFE  570
            GOTO319                                                                 FFE  571
C                                                                                   FFE  572
C           COMPUTE FOR ALL PRINCIPAL AXES, ALL REFERENCE AXES,                     FFE  573
C                                                  AND ALL ATOMS                    FFE  574
  311       NA#IN(2)                                                              FFE  575
            DO317I#1,NA                                                             FFE  576
                                                                                    FFE  577
               IN(2)#I                                                              FFE  578
  317          CALLSUB11                                                          FFE  579
                                                                                    FFE  580
  319 RETURN                                                                        FFE  581
      END(0,1,0,0,0)                                                              FFE  582
*TYPE(FORTRAN)                                                                     FFE  583
C     SELECT THE HED SUBROUTINE TO BE ENTERED                                     FFE  584
      SUBROUTINE HED1(I)                                                          FFE  585
      K#XMODF(I,100)                                                              FFE  586
      IF(K)160,160,4                                                              FFE  587
                                                                                    FFE  588
    4 IF(K-15)8,8,160                                                           FFE  589
                                                                                    FFE  590
    8 GO TO (10,20,30,40,50,60,70,80,90,100,110,120,130,140,150),K                  FFE  591
                                                                                    FFE  592
   10    CALL HED1                                                                FFE  593
         GO TO 160                                                                  FFE  594
                                                                                    FFE  595
   20    CALL HED2                                                                FFE  596
         GO TO 160                                                                  FFE  597
                                                                                    FFE  598
   30    CALL HED3                                                                FFE  599
         GO TO 160                                                                  FFE  600
                                                                                    FFE  601
   40    CALL HED4                                                                FFE  602
         GO TO 160                                                                  FFE  603
                                                                                    FFE  604
   50    CALL HED5                                                                FFE  605
         GO TO 160                                                                  FFE  606
                                                                                    FFE  607
   60    CALL HED6                                                                FFE  608
         GO TO 160                                                                  FFE  609
                                                                                    FFE  610
   70    CALL HED7                                                                FFE  611
         GO TO 160                                                                  FFE  612
                                                                                    FFE  613
   80    CALL HED8                                                                FFE  614
         GO TO 160                                                                  FFE  615
                                                                                    FFE  616
   90    CALL HED9                                                                FFE  617
         GO TO 160                                                                  FFE  618
                                                                                    FFE  619
  100    CALL HED10                                                               FFE  620
         GO TO 160                                                                  FFE  621
                                                                                    FFE  622
  110    CALL HED11                                                               FFE  623
         GO TO 160                                                                  FFE  624
                                                                                    FFE  625
  120    CALL HED12                                                               FFE  626
         GO TO 160                                                                  FFE  626
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                                                                        FFE  627
  130     CALL HED13                                                    FFE  628
          GO TO 160                                                     FFE  629
                                                                        FFE  630
  140     CALL HED14                                                    FFE  631
          GO TO 160                                                     FFE  632
                                                                        FFE  633
  150     CALL HED15                                                    FFE  634
                                                                        FFE  635
  160 RETURN                                                            FFE  636
      END(0,1,0,0,0)                                                    FFE  637
*TYPE (FORTRAN)                                                         FFE  638
C     SELECT THE PRE SUBROUTINE TO BE ENTERED                           FFE  639
      SUBROUTINE PREI(I)                                                FFE  640
    4 IF(I)160,160,6                                                    FFE  641
                                                                        FFE  642
    6 IF(I-15)8,8,160                                                   FFE  643
                                                                        FFE  644
    8 GO TO (10,20,30,40,50,60,70,80,80,100,100,120,70,140,140),I       FFE  645
                                                                        FFE  646
   10     CALL PRE1                                                    FFE  647
          GO TO 160                                                     FFE  648
                                                                        FFE  649
   20     CALL PRE2                                                    FFE  650
          GO TO 160                                                     FFE  651
                                                                        FFE  652
   30     CALL PRE3                                                    FFE  653
          GO TO 160                                                     FFE  654
                                                                        FFE  655
   40     CALL PRE4                                                    FFE  656
          GO TO 160                                                     FFE  657
                                                                        FFE  658
   60     CALL PRE6                                                    FFE  659
          GO TO 160                                                     FFE  660
                                                                        FFE  661
   70     CALL PRE7                                                    FFE  662
          GO TO 160                                                     FFE  663
                                                                        FFE  664
   80     CALL PRE8                                                    FFE  665
          GO TO 160                                                     FFE  666
                                                                        FFE  667
                                                                        FFE  668
  100     CALL PRE10                                                    FFE  669
          GO TO 160                                                     FFE  670
                                                                        FFE  671
  120     CALL PRE12                                                    FFE  672
          GO TO 160                                                     FFE  673
                                                                        FFE  674
  140     CALL PRE14                                                    FFE  675
                                                                        FFE  676
  160 RETURN                                                            FFE  677
      END(0,1,0,0,0)                                                    FFE  678
*TYPE (FORTRAN)                                                         FFE  679
C     SELECT THE FUN SUBROUTINE TO BE ENTERED                           FFE  680
      SUBROUTINE FUNI(I)                                                FFE  681
                                                                        FFE  682
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  683
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVFA,SAVFP,VARA,VARP,FI,F,IH,NSP  FFE  684
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  685
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE  686
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  687
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  688
                                                                        FFE  689
      CALL SETA(A)                                                      FFE  690
      CALL SETP(P)                                                      FFE  691
      IF(I)6,6,5                                                        FFE  692
                                                                        FFE  693
    5 IF(I-15)8,8,6                                                     FFE  694
                                                                        FFE  695
    6     NG#11                                                         FFE  696
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            GO TO 160                                                          FFE  697
                                                                               FFE  698
          8 GO TO (10,20,30,40,50,60,70,80,90,100,110,120,130,140,150),I       FFE  699
                                                                               FFE  700
         10     CALL FUN1                                                      FFE  701
                GO TO 160                                                      FFE  702
                                                                               FFE  703
         20     CALL FUN2                                                      FFE  704
                GO TO 160                                                      FFE  705
                                                                               FFE  706
         30     CALL FUN3                                                      FFE  707
                GO TO 160                                                      FFE  708
                                                                               FFE  709
         40     CALL FUN4                                                      FFE  710
                GO TO 160                                                      FFE  711
                                                                               FFE  712
         50     CALL FUN5                                                      FFE  713
                GO TO 160                                                      FFE  714
                                                                               FFE  715
         60     CALL FUN6                                                      FFE  716
                GO TO 160                                                      FFE  717
                                                                               FFE  718
         70     CALL FUN7                                                      FFE  719
                GO TO 160                                                      FFE  720
                                                                               FFE  721
         80     CALL FUN8                                                      FFE  722
                GO TO 160                                                      FFE  723
                                                                               FFE  724
         90     CALL FUN9                                                      FFE  725
                GO TO 160                                                      FFE  726
                                                                               FFE  727
        100     CALL FUN10                                                     FFE  728
                GO TO 160                                                      FFE  729
                                                                               FFE  730
        110     CALL FUN11                                                     FFE  731
                GO TO 160                                                      FFE  732
                                                                               FFE  733
        120     CALL FUN12                                                     FFE  734
                GO TO 160                                                      FFE  735
                                                                               FFE  736
        130     CALL FUN13                                                     FFE  737
                GO TO 160                                                      FFE  738
                                                                               FFE  739
        140     CALL FUN14                                                     FFE  740
                GO TO 160                                                      FFE  741
                                                                               FFE  742
        150     CALL FUN15                                                     FFE  743
                                                                               FFE  744
        160 RETURN                                                             FFE  745
            END(0,1,0,0,0)                                                     FFE  746
    *TYPE (FORTRAN)                                                            FFE  747
    C       SELECT THE OUT SUBROUTINE TO BE ENTERED                            FFE  748
            SUBROUTINE OUTI(I)                                                 FFE  749
          4 IF(I)160,160,6                                                     FFE  750
                                                                               FFE  751
          6 IF(I-15)8,8,160                                                    FFE  752
                                                                               FFE  753
          8 GO TO (10,20,30,40,50,60,70,80,90,100,110,120,130,10,10),I         FFE  754
                                                                               FFE  755
         10     CALL OUT1                                                      FFE  756
                GO TO 160                                                      FFE  757
                                                                               FFE  758
         20     CALL OUT2                                                      FFE  759
                GO TO 160                                                      FFE  760
                                                                               FFE  761
         30     CALL OUT3                                                      FFE  762
                GO TO 160                                                      FFE  763
                                                                               FFE  764
         40     CALL OUT4                                                      FFE  765
                GO TO 160                                                      FFE  766
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                                                                      FFE  767
   60     CALL OUT6                                                   FFE  768
          GO TO 160                                                   FFE  769
                                                                      FFE  770
   70     CALL OUT7                                                   FFE  771
          GO TO 160                                                   FFE  772
                                                                      FFE  773
   80     CALL OUT8                                                   FFE  774
          GO TO 160                                                   FFE  775
                                                                      FFE  776
  100     CALL OUT10                                                  FFE  777
          GO TO 160                                                   FFE  778
                                                                      FFE  779
  120     CALL OUT12                                                  FFE  780
          GO TO 160                                                   FFE  781
                                                                      FFE  782
  130     CALL OUT13                                                  FFE  783
                                                                      FFE  784
  160 RETURN                                                          FFE  785
      END(0,1,0,0,0)                                                  FFE  786
*TYPE(FORTRAN)                                                        FFE  787
C     SET KEY WORDS FOR ATOM COORDINATES                              FFE  788
      SUBROUTINE SETKX(I)                                             FFE  789
C     I#IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER     FFE  790
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE FFE  791
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP FFE  792
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  793
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)    FFE  794
      DIMENSION DFDA(6),IN(2311),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  795
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                       FFE  796
      IF(I)119,119,111                                                FFE  797
  111 J#JX+JXP*(I-1)                                                  FFE  798
      KI2(J)#I                                                        FFE  799
      KI2(J+1)#I                                                      FFE  800
      KI2(J+2)#I                                                      FFE  801
  119 RETURN                                                          FFE  802
      END(0,1,0,0,0)                                                  FFE  803
*TYPE(FORTRAN)                                                        FFE  804
C     SET KEY WORDS FOR ATOM BETAS                                    FFE  805
      SUBROUTINE SETKB(I)                                             FFE  806
C     I#IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER     FFE  807
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE FFE  808
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP FFE  809
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  810
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)    FFE  811
      DIMENSION DFDA(6),IN(2311),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  812
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                       FFE  813
      IF(I)119,119,111                                                FFE  814
  111 J#JB+JBP*(I-1)                                                  FFE  815
      DO 117 K#1,6                                                    FFE  816
      KI2(J)#I                                                        FFE  817
  117 J#J+1                                                           FFE  818
  119 RETURN                                                          FFE  819
      END(0,1,0,0,0)                                                  FFE  820
*TYPE(FORTRAN)                                                        FFE  821
C     STORE METRIC TENSOR                                             FFE  822
      SUBROUTINE STOAA                                                FFE  823
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE FFE  824
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP FFE  825
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  826
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)    FFE  827
      DIMENSION DFDA(6),IN(2311),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  828
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                       FFE  829
      AA(1,1)#A(1)*A(1)                                               FFE  830
      AA(2,2)#A(2)*A(2)                                               FFE  831
      AA(3,3)#A(3)*A(3)                                               FFE  832
      AA(1,2)#A(1)*A(2)*A(6)                                          FFE  833
      AA(2,1)#AA(1,2)                                                 FFE  834
      AA(1,3)#A(1)*A(3)*A(5)                                          FFE  835
      AA(3,1)#AA(1,3)                                                 FFE  836
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      AA(2,3)#A(2)*A(3)*A(4)                                                    FFE  837
      AA(3,2)#AA(2,3)                                                           FFE  838
      RETURN                                                                    FFE  839
      END(0,1,0,0,0)                                                            FFE  840
*TYPE(FORTRAN)                                                                  FFE  841
C     STORE RECIPROCAL METRIC TENSOR                                            FFE  842
      SUBROUTINE STOBB                                                          FFE  843
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE           FFE  844
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP          FFE  845
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2         FFE  846
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)              FFE  847
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  848
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                                 FFE  849
      DIMENSIONAI(6),CI(6),BBII(3),BBJK(3)                                      FFE  850
      DO12II#1,3                                                                FFE  851
      IF(A(I))111,111,115                                                       FFE  852
  111 NG#6                                                                      FFE  853
      GOTO225                                                                   FFE  854
  115 AI(I)#A(I)                                                                FFE  855
      AI(I+3)#A(I)                                                              FFE  856
      CI(I)#A(I+3)                                                              FFE  857
  121 CI(I+3)#A(I+3)                                                            FFE  858
      X#1.0/(AI(1)*AI(2)*AI(3)*(1.0-CI(1)*CI(1)-CI(2)*CI(2)                     FFE  859
     1-CI(3)*CI(3)+2.0*CI(1)*CI(2)*CI(3)))                                      FFE  860
      DO205I#1,3                                                                FFE  861
      BBII(I)#X*(1.0-CI(I)*CI(I))*AI(I+1)*AI(I+2)/AI(I)                         FFE  862
  205 BBJK(I)#X*AI(I)*(CI(I+1)*CI(I+2)-CI(I))                                   FFE  863
      BB(1,1)#BBII(1)                                                           FFE  864
      BB(1,2)#BBJK(3)                                                           FFE  865
      BB(1,3)#BBJK(2)                                                           FFE  866
      BB(2,1)#BBJK(3)                                                           FFE  867
      BB(2,2)#BBII(2)                                                           FFE  868
      BB(2,3)#BBJK(1)                                                           FFE  869
      BB(3,1)#BBJK(2)                                                           FFE  870
      BB(3,2)#BBJK(1)                                                           FFE  871
      BB(3,3)#BBII(3)                                                           FFE  872
  225 RETURN                                                                    FFE  873
      END(0,1,0,0,0)                                                            FFE  874
*TYPE(FORTRAN)                                                                  FFE  875
C     ATOM COORDINATE SUBROUTINE                                                FFE  876
      SUBROUTINE ATOM(I,Z)                                                      FFE  877
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE           FFE  878
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP          FFE  879
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2         FFE  880
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)              FFE  881
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  882
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                                 FFE  883
      DIMENSIONI(2),X(3),Y(3),Z(3)                                              FFE  884
      IF(I(1))109,109,117                                                       FFE  885
  109 X(1)#0.0                                                                  FFE  886
      X(2)#0.0                                                                  FFE  887
      X(3)#0.0                                                                  FFE  888
      GOTO125                                                                   FFE  889
  117 K#JXP*(I(1)-1)+JX                                                         FFE  890
      IF(K+2-NP)119,119,503                                                     FFE  891
  503 NG#5                                                                      FFE  892
      GOTO325                                                                   FFE  893
  119 DO123J#1,3                                                                FFE  894
      X(J)#P(K)                                                                 FFE  895
  123 K#K+1                                                                     FFE  896
  125 KC#I(2)/100                                                               FFE  897
      KS#I(2)-100*KC                                                            FFE  898
      IF(KS-NS)203,203,403                                                      FFE  899
  403 NG#1                                                                      FFE  900
      GOTO325                                                                   FFE  901
  203 IF(KS)403,205,213                                                         FFE  902
  205 Y(1)#X(1)                                                                 FFE  903
      Y(2)#X(2)                                                                 FFE  904
      Y(3)#X(3)                                                                 FFE  905
      GOTO311                                                                   FFE  906
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  213 DO215J#1,3                                                        FFE  907
  215 Y(J)#TS(J,KS)                                                     FFE  908
      DO309K#1,3                                                        FFE  909
      DO307J#1,2                                                        FFE  910
      L#IS(J,K,KS)                                                      FFE  911
      IF(L)225,307,305                                                  FFE  912
  225 L#-L                                                              FFE  913
      Y(K)#Y(K)-X(L)                                                    FFE  914
      GOTO307                                                           FFE  915
  305 Y(K)#Y(K)+X(L)                                                    FFE  916
  307 CONTINUE                                                          FFE  917
  309 CONTINUE                                                          FFE  918
  311 KC4#KC/4                                                          FFE  919
      KC3#KC-4*KC4                                                      FFE  920
      KC2#KC3/2                                                         FFE  921
      KC1#KC3-2*KC2                                                     FFE  922
      Z(1)#Y(1)-FLOATF(KC1)                                             FFE  923
      Z(2)#Y(2)-FLOATF(KC2)                                             FFE  924
      Z(3)#Y(3)-FLOATF(KC4)                                             FFE  925
  325 RETURN                                                            FFE  926
      END(0,1,0,0,0)                                                    FFE  927
*TYPE(FORTRAN)                                                          FFE  928
C     STORE TRANSFORMED ANISOTROPIC TEMP FACTOR MATRIX                  FFE  929
C     INS IS ATOM DESCRIPTION, Z IS TRANSFORMED MATRIX                  FFE  930
      SUBROUTINE BETA(INS,Z)                                            FFE  931
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE  932
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP  FFE  933
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE  934
      DIMENSION TITLE(12),PM(201,100),DP(200),DFDP(200),AM(21),DA(6)    FFE  935
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE  936
      )IMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE  937
      DIMENSIONINS(2),Z(3,3),B1(6),B2(9)                                FFE  938
      IF(ITF-1)100,111,115                                              FFE  939
  100 IF(JBP-6)111,115,115                                              FFE  940
  111 NG#4                                                              FFE  941
      GOTO423                                                           FFE  942
  115 KS#XMODF(INS(2),100)                                              FFE  943
      IF(KS)121,119,119                                                 FFE  944
  119 IF(KS-NS)125,125,121                                              FFE  945
  121 NG#1                                                              FFE  946
      GOTO423                                                           FFE  947
  125 IF(INS(1))211,201,207                                             FFE  948
  201 DO203I#1,6                                                        FFE  949
  203 B1(I)#0.0                                                         FFE  950
      GOTO221                                                           FFE  951
  207 J#JB+JBP*(INS(1)-1)                                               FFE  952
      IF(J+5-NP)215,215,211                                             FFE  953
  211 NG#5                                                              FFE  954
      GOTO423                                                           FFE  955
  215 DO219I#1,6                                                        FFE  956
      B1(I)#P(J)                                                        FFE  957
  219 J#J+1                                                             FFE  958
  221 B2(1)#B1(1)                                                       FFE  959
      B2(2)#B1(4)                                                       FFE  960
      B2(3)#B1(5)                                                       FFE  961
      B2(4)#B1(2)                                                       FFE  962
      B2(6)#B1(6)                                                       FFE  963
      B2(9)#B1(3)                                                       FFE  964
      DO421I#1,3                                                        FFE  965
      DO419J#1,3                                                        FFE  966
      IF(KS)121,313,319                                                 FFE  967
  313 M#I*J                                                             FFE  968
      B3#B2(M)                                                          FFE  969
      GOTO415                                                           FFE  970
  319 B3#0.0                                                            FFE  971
      DO413K#1,2                                                        FFE  972
      DO411L#1,2                                                        FFE  973
      M#IS(K,I,KS)*IS(L,J,KS)                                           FFE  974
      IF(M)407,411,403                                                  FFE  975
  403 B3#B3+B2(M)                                                       FFE  976
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      GOTO411                                                          FFE  977
  407 M#-M                                                             FFE  978
      B3#B3-B2(M)                                                      FFE  979
  411 CONTINUE                                                         FFE  980
  413 CONTINUE                                                         FFE  981
  415 Z(I,J)#B3                                                        FFE  982
      Z(J,I)#B3                                                        FFE  983
  419 CONTINUE                                                         FFE  984
  421 CONTINUE                                                         FFE  985
  423 RETURN                                                           FFE  986
      END(0,1,0,0,0)                                                   FFE  987
*TYPE(FORTRAN)                                                         FFE  988
C     MULTIPLY TWO MATRICES                                            FFE  989
C     Z(3,3)#X(3,3)*Y(3,3)                                             FFE  990
      SUBROUTINE MM(X,Y,Z)                                             FFE  991
      DIMENSIONX(3,3),Y(3,3),Z(3,3)                                    FFE  992
      DO117I#1,3                                                       FFE  993
      DO117K#1,3                                                       FFE  994
      Z(I,K)#0.0                                                       FFE  995
      DO117J#1,3                                                       FFE  996
  117 Z(I,K)#Z(I,K)+X(I,J)*Y(J,K)                                      FFE  997
      RETURN                                                           FFE  998
      END(0,1,0,0,0)                                                   FFE  999
*TYPE(FORTRAN)                                                         FFE 1000
C     MATRIX * VECTOR                                                  FFE 1001
C     Z(3)#X(3,3)*Y(3)                                                 FFE 1002
      SUBROUTINE MV(X,Y,Z)                                             FFE 1003
      DIMENSIONX(3,3),Y(3),Z(3)                                        FFE 1004
      DO113I#1,3                                                       FFE 1005
      Z(I)#0.0                                                         FFE 1006
      DO113J#1,3                                                       FFE 1007
  113 Z(I)#Z(I)+X(I,J)*Y(J)                                            FFE 1008
      RETURN                                                           FFE 1009
      END(0,1,0,0,0)                                                   FFE 1010
*TYPE(FORTRAN)                                                         FFE 1011
C     TRANSPOSED VECTOR TIMES MATRIX                                   FFE 1012
C     Z(3)#X(3)*Y(3,3)                                                 FFE 1013
      SUBROUTINE VM(X,Y,Z)                                             FFE 1014
      )IMENSIONX(3),Y(3,3),Z(3)                                        FFE 1015
      DO115J#1,3                                                       FFE 1016
      Z(J)#0.0                                                         FFE 1017
      DO115I#1,3                                                       FFE 1018
  115 Z(J)#Z(J)+X(I)*Y(I,J)                                            FFE 1019
      RETURN                                                           FFE 1020
      END(0,1,0,0,0)                                                   FFE 1021
*TYPE(FORTRAN)                                                         FFE 1022
C     TRANSPOSED VECTOR * VECTOR                                       FFE 1023
C     VV#X(3)*Y(3)                                                     FFE 1024
      FUNCTION VV(X,Y)                                                 FFE 1025
      DIMENSIONX(3),Y(3)                                               FFE 1026
      VV#0.0                                                           FFE 1027
      DO111I#1,3                                                       FFE 1028
  111 VV#VV+X(I)*Y(I)                                                  FFE 1029
      RETURN                                                           FFE 1030
      END(0,1,0,0,0)                                                   FFE 1031
*TYPE(FORTRAN)                                                         FFE 1032
C     TRANSPOSED VECTOR * MATRIX * VECTOR                              FFE 1033
C     VMV#W(3)*X(3,3)*Y(3)                                             FFE 1034
      FUNCTION VMV(W,X,Y)                                              FFE 1035
      DIMENSIONW(3),X(3,3),Y(3),Z(3)                                   FFE 1036
      CALLMV(X,Y,Z)                                                    FFE 1037
      VMV#VV(W,Z)                                                      FFE 1038
      RETURN                                                           FFE 1039
      END(0,1,0,0,0)                                                   FFE 1040
*TYPE(FORTRAN)                                                         FFE 1041
C     VECTOR - VECTOR                                                  FFE 1042
C     Z(3)#X(3)-Y(3)                                                   FFE 1043
      SUBROUTINE DIFV(X,Y,Z)                                           FFE 1044
      DIMENSIONX(3),Y(3),Z(3)                                          FFE 1045
      DO111I#1,3                                                       FFE 1046
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  111 Z(I)#X(I)-Y(I)                                                    FFE 1047
      RETURN                                                            FFE 1048
      END(0,1,0,0,0)                                                    FFE 1049
*TYPE(FORTRAN)                                                          FFE 1050
C     COMPUTE THE SUM OF TWO VECTORS                                    FFE 1051
C     Z(3)#X(3)+Y(3)                                                    FFE 1052
      SUBROUTINE SUMV(X,Y,Z)                                            FFE 1053
      )IMENSIONX(3),Y(3),Z(3)                                           FFE 1054
      DO1111#1,3                                                        FFE 1055
  111 Z(I)#X(I)+Y(I)                                                    FFE 1056
      RETURN                                                            FFE 1057
      END(0,1,0,0,0)                                                    FFE 1058
*TYPE(FORTRAN)                                                          FFE 1059
C     COSINE OF ANGLE BETWEEN VECTORS X AND Y                           FFE 1060
      FUNCTION COSVV(X,Y)                                               FFE 1061
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1062
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1063
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1064
      DIMENSION TITLE(12),PM(2100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1065
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1066
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1067
      DIMENSIONX(3),Y(3)                                                FFE 1068
      D#SQRTF(VMV(X,AA,X)*VMV(Y,AA,Y))                                  FFE 1069
      IF(D)111,111,115                                                  FFE 1070
  111 NG#9                                                              FFE 1071
      GOTO117                                                           FFE 1072
  115 COSVV#VMV(X,AA,Y)/D                                               FFE 1073
  117 RETURN                                                            FFE 1074
      END(0,1,0,0,0)                                                    FFE 1075
*TYPE(FORTRAN)                                                          FFE 1076
C     ARCCOS(X) IN DEGREES                                              FFE 1077
      FUNCTION ARCCOS(X)                                                FFE 1078
      ARCCOS#90.0-(57.29577951)*SIGNF(ASINF(X),X)                       FFE 1079
      RETURN                                                            FFE 1080
      END(0,1,0,0,0)                                                    FFE 1081
*TYPE(FORTRAN)                                                          FFE 1082
C     STORE A VECTOR Z NORMAL TO VECTORS X AND Y                        FFE 1083
      SUBROUTINE NORM(X,Y,Z)                                            FFE 1084
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1085
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1086
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1087
      DIMENSION TITLE(12),PM(2100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1088
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1089
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1090
      DIMENSIONX(3),Y(3),Z(3),XI(6),YI(6),ZI(3)                         FFE 1091
      DO115I#1,3                                                        FFE 1092
      XI(I)#X(I)                                                        FFE 1093
      XI(I+3)#X(I)                                                      FFE 1094
      YI(I)#Y(I)                                                        FFE 1095
  115 YI(I+3)#Y(I)                                                      FFE 1096
      DO119I#1,3                                                        FFE 1097
  119 ZI(I)#XI(I+1)*YI(I+2)-XI(I+2)*YI(I+1)                             FFE 1098
      CALLMV(BB,ZI,Z)                                                   FFE 1099
      RETURN                                                            FFE 1100
      END(0,1,0,0,0)                                                    FFE 1101
*TYPE(FORTRAN)                                                          FFE 1102
C     STORE THREE MUTUALLY PERPENDICULAR                                FFE 1103
C        VECTORS X(I,1), X(I,2), AND X(I,3) GIVEN                       FFE 1104
C        VECTORS U AND V.                                               FFE 1105
      SUBROUTINE AXES(U,V,X)                                            FFE 1106
      DIMENSIONU(3),V(3),X(3,3)                                         FFE 1107
      DO113I#1,3                                                        FFE 1108
  113 X(I,1)#U(I)                                                       FFE 1109
      CALLNORM(U,V,X(1,2))                                              FFE 1110
      CALLNORM(X(1,1),X(1,2),X(1,3))                                    FFE 1111
      RETURN                                                            FFE 1112
      END(0,1,0,0,0)                                                    FFE 1113
*TYPE(FORTRAN)                                                          FFE 1114
C     FIND EIGENVALUES Y OF MATRIX W                                    FFE 1115
      SUBROUTINE EIGVAL(W,Y)                                            FFE 1116
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      COMMONNG                                                          FFE 1117
      DIMENSIONW(3,3),Y(3),X(3),Z(6,6)                                  FFE 1118
      DO119J#1,3                                                        FFE 1119
      DO119I#1,3                                                        FFE 1120
      ZI#W(I,J)                                                         FFE 1121
      Z(I,J)#ZI                                                         FFE 1122
      Z(I+3,J)#ZI                                                       FFE 1123
      Z(I,J+3)#ZI                                                       FFE 1124
  119 Z(I+3,J+3)#ZI                                                     FFE 1125
      P#0.0                                                             FFE 1126
      Q#0.0                                                             FFE 1127
      R#0.0                                                             FFE 1128
      DO207I#1,3                                                        FFE 1129
      P#P-Z(I,I)                                                        FFE 1130
      Q#Q+Z(I,I)*Z(I+1,I+1)-Z(I,I+1)*Z(I+1,I)                           FFE 1131
  207 R#R+Z(3,I)*Z(2,I+1)*Z(1,I+2)-Z(1,I)*Z(2,I+1)*Z(3,I+2)             FFE 1132
      P3#P/3.0                                                          FFE 1133
      A#Q-P*P3                                                          FFE 1134
      B#2.0*P3*P3*P3-Q*P3+R                                             FFE 1135
      B2#B/2.0                                                          FFE 1136
      A3#A/3.0                                                          FFE 1137
      B4#B2*B2                                                          FFE 1138
      A27#A3*A3*A3                                                      FFE 1139
      IF(B4+A27)303,303,215                                             FFE 1140
  215 IF(B4+1.0001*A27)220,220,225                                      FFE 1141
  220 A27#-B4                                                           FFE 1142
      GOTO303                                                           FFE 1143
  225 NG#7                                                              FFE 1144
      GOTO317                                                           FFE 1145
  303 PHI3#(ASINF(SQRTF(1.0+(B4/A27))))/3.0                             FFE 1146
      IF(B)307,305,307                                                  FFE 1147
  305 B#0.0                                                             FFE 1148
  307 C#-SIGNF((2.0*SQRTF(-A3)),B)                                      FFE 1149
      X(1)#C*COSF(PHI3)                                                 FFE 1150
      X(2)#C*COSF(PHI3+4.188790205)                                     FFE 1151
      X(3)#C*COSF(PHI3+2.094395103)                                     FFE 1152
      IF(B)311,313,313                                                  FFE 1153
  311 HOLD#X(1)                                                         FFE 1154
      X(1)#X(3)                                                         FFE 1155
      X(3)#HOLD                                                         FFE 1156
  313 DO315I#1,3                                                        FFE 1157
  315 Y(I)#X(I)-P3                                                      FFE 1158
  317 RETURN                                                            FFE 1159
      END(0,1,0,0,0)                                                    FFE 1160
*TYPE(FORTRAN)                                                          FFE 1161
C     COMPUTE EIGENVECTOR Z OF MATRIX                                   FFE 1162
C        W GIVEN EIGENVALUE Y                                           FFE 1163
      SUBROUTINE EIGVEC(W,Y,Z)                                          FFE 1164
      COMMONNG                                                          FFE 1165
      DIMENSIONW(3,3),X(6,6),Z(3),P(3)                                  FFE 1166
      DO123J#1,3                                                        FFE 1167
      DO123I#1,3                                                        FFE 1168
      XI#W(I,J)                                                         FFE 1169
      X(I,J)#XI                                                         FFE 1170
      ((I+3,J)#XI                                                       FFE 1171
      X(I,J+3)#XI                                                       FFE 1172
  123 X(I+3,J+3)#XI                                                     FFE 1173
      YI#Y                                                              FFE 1174
      DO209I#1,3                                                        FFE 1175
      X(I,I)#X(I,I)-YI                                                  FFE 1176
      X(I+3,I)#X(I+3,I)-YI                                              FFE 1177
      X(I,I+3)#X(I,I+3)-YI                                              FFE 1178
  209 X(I+3,I+3)#X(I+3,I+3)-YI                                          FFE 1179
      SI#0.0                                                            FFE 1180
      DO307I#1,3                                                        FFE 1181
      S#0.0                                                             FFE 1182
      DO223J#1,3                                                        FFE 1183
      PJ#X(I,J+1)*X(I+1,J+2)-X(I,J+2)*X(I+1,J+1)                        FFE 1184
      P(J)#PJ                                                           FFE 1185
  223 S#S+PJ*PJ                                                         FFE 1186
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      IF(S-SI)307,307,301                                                FFE 1187
  301 SI#S                                                               FFE 1188
      DO305J#1,3                                                         FFE 1189
  305 Z(J)#P(J)                                                          FFE 1190
  307 CONTINUE                                                           FFE 1191
      IF(SI)311,311,313                                                  FFE 1192
  311 NG#8                                                               FFE 1193
  313 RETURN                                                             FFE 1194
      END(0,1,0,0,0)                                                     FFE 1195
*TYPE(FORTRAN)                                                           FFE 1196
C     COMPUTE TRACE OF MATRIX X                                          FFE 1197
      FUNCTION TRACE(X)                                                  FFE 1198
      DIMENSIONX(3,3)                                                    FFE 1199
      TRACE#0.0                                                          FFE 1200
      DO111I#1,3                                                         FFE 1201
  111 TRACE#TRACE+X(I,I)                                                 FFE 1202
      RETURN                                                             FFE 1203
      END(0,1,0,0,0)                                                     FFE 1204
*TYPE(FORTRAN)                                                           FFE 1205
C     ANGLE SUBROUTINE USED BY FUN2, FUN5, FUN6                          FFE 1206
      FUNCTION FUNA(I)                                                   FFE 1207
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1208
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE 1209
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1210
      DIMENSION TITLE(12),PM(201,00),DP(200),DFDP(200),AM(21),DA(6)      FFE 1211
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1212
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1213
      DIMENSIONI(6),X1(3),X2(3),X3(3),V1(3),V2(3)                        FFE 1214
      CALLSTOAA                                                          FFE 1215
      CALLATOM(I(1),X1)                                                  FFE 1216
      CALLATOM(I(3),X2)                                                  FFE 1217
      CALLATOM(I(5),X3)                                                  FFE 1218
      IF(NG)123,117,123                                                  FFE 1219
  117 CALLDIFV(X1,X2,V1)                                                 FFE 1220
      CALLDIFV(X3,X2,V2)                                                 FFE 1221
      FUNA#ARCCOS(COSVV(V1,V2))                                          FFE 1222
  123 RETURN                                                             FFE 1223
      END(0,1,0,0,0)                                                     FFE 1224
*TYPE(FORTRAN)                                                           FFE 1225
C     DISTANCE SUBROUTINE USED BY FUN1 AND FUN4                          FFE 1226
      FUNCTION FUND(I)                                                   FFE 1227
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1228
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE 1229
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1230
      DIMENSION TITLE(12),PM(201,00),DP(200),DFDP(200),AM(21),DA(6)      FFE 1231
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1232
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1233
      DIMENSIONI(4),X1(3),X2(3),V(3)                                     FFE 1234
      CALLSTOAA                                                          FFE 1235
      CALLATOM(I(1),X1)                                                  FFE 1236
      CALLATOM(I(3),X2)                                                  FFE 1237
      CALLDIFV(X2,X1,V)                                                  FFE 1238
      FUND#SQRTF(VMV(V,AA,V))                                            FFE 1239
      RETURN                                                             FFE 1240
      END(0,1,0,0,0)                                                     FFE 1241
*TYPE(FORTRAN)                                                           FFE 1242
C     HEADING 1                                                          FFE 1243
      SUBROUTINE HED1                                                    FFE 1244
      WRITEOUTPUTTAPE9,107                                               FFE 1245
  107 FORMAT(34HOINTERATOMIC DISTANCE IN ANGSTROMS)                      FFE 1246
      RETURN                                                             FFE 1247
      END(0,1,0,0,0)                                                     FFE 1248
*TYPE(FORTRAN)                                                           FFE 1249
C     SET KEY WORDS FOR INTERATOMIC DISTANCE                             FFE 1250
      SUBROUTINE PRE1                                                    FFE 1251
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1252
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE 1253
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1254
      DIMENSION TITLE(12),PM(201,00),DP(200),DFDP(200),AM(21),DA(6)      FFE 1255
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1256
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      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1257
      CALLSETKX(IN(2))                                                   FFE 1258
      CALLSETKX(IN(4))                                                   FFE 1259
      RETURN                                                             FFE 1260
      END(0,1,0,0,0)                                                     FFE 1261
*TYPE(FORTRAN)                                                           FFE 1262
C     COMPUTE INTERATOMIC DISTANCE                                       FFE 1263
      SUBROUTINE FUN1                                                    FFE 1264
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1265
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP   FFE 1266
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1267
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1268
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1269
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1270
      FX#FUND(IN(2))                                                     FFE 1271
      RETURN                                                             FFE 1272
      END(0,1,0,0,0)                                                     FFE 1273
*TYPE(FORTRAN)                                                           FFE 1274
C     PUT OUT DESCRIPTION OF INTERATOMIC DISTANCE                        FFE 1275
      SUBROUTINE OUT1                                                    FFE 1276
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1277
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP   FFE 1278
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1279
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1280
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1281
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1282
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,5)                                 FFE 1283
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,1H))                  FFE 1284
      RETURN                                                             FFE 1285
      END(0,1,0,0,0)                                                     FFE 1286
*TYPE(FORTRAN)                                                           FFE 1287
C     HEADING 2                                                          FFE 1288
      SUBROUTINE HED2                                                    FFE 1289
      WRITE OUTPUT TAPE 9,107                                            FFE 1290
  107 FORMAT(46H0BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX)          FFE 1291
      RETURN                                                             FFE 1292
      END(0,1,0,0,0)                                                     FFE 1293
*TYPE(FORTRAN)                                                           FFE 1294
C     PRELIMINARY SUBROUTINE 2                                           FFE 1295
      SUBROUTINE PRE2                                                    FFE 1296
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1297
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP   FFE 1298
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1299
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1300
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1301
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1302
      DO107I#2,6,2                                                       FFE 1303
  107 CALLSETKX(IN(I))                                                   FFE 1304
      RETURN                                                             FFE 1305
      END(0,1,0,0,0)                                                     FFE 1306
*TYPE(FORTRAN)                                                           FFE 1307
C     BOND ANGLE SUBROUTINE                                              FFE 1308
      SUBROUTINE FUN2                                                    FFE 1309
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1310
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP   FFE 1311
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1312
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1313
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1314
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1315
      FX#FUNA(IN(2))                                                     FFE 1316
      RETURN                                                             FFE 1317
      END(0,1,0,0,0)                                                     FFE 1318
*TYPE(FORTRAN)                                                           FFE 1319
C     OUTPUT DESCRIPTION 2                                               FFE 1320
      SUBROUTINE OUT2                                                    FFE 1321
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1322
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP   FFE 1323
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1324
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1325
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1326
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      )IMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1327
      WRITE OUTPUT TAPE 9,107,(IN(I),I#2,7)                              FFE 1328
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H))    FFE 1329
      RETURN                                                             FFE 1330
      END(0,1,0,0,0)                                                     FFE 1331
*TYPE(FORTRAN)                                                           FFE 1332
C     HEADING 3                                                          FFE 1333
      SUBROUTINE HED3                                                    FFE 1334
      WRITE OUTPUT TAPE 9,107                                            FFE 1335
  107 FORMAT(58H0DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOFFE 1336
     1MS)                                                                FFE 1337
      RETURN                                                             FFE 1338
      END(0,1,0,0,0)                                                     FFE 1339
*TYPE(FORTRAN)                                                           FFE 1340
C     PRELIMINARY SUBROUTINE 3                                           FFE 1341
      SUBROUTINE PRE3                                                    FFE 1342
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1343
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE 1344
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1345
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1346
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1347
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1348
      DO1071#2,12,2                                                      FFE 1349
  107 CALLSETKX(IN(I),)                                                  FFE 1350
      RETURN                                                             FFE 1351
      END(0,1,0,0,0)                                                     FFE 1352
*TYPE(FORTRAN)                                                           FFE 1353
C     DIHEDRAL ANGLE SUBROUTINE                                          FFE 1354
      SUBROUTINE FUN3                                                    FFE 1355
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1356
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE 1357
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1358
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1359
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1360
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1361
      DIMENSIONX(3,6),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3)                FFE 1362
      CALLSTOAA                                                          FFE 1363
      CALLSTOBB                                                          FFE 1364
      IF(NG)207,113,207                                                  FFE 1365
  113 DO115I#1,6                                                         FFE 1366
  115 CALLATOM(IN(2*I),X(1,I))                                           FFE 1367
      IF(NG)207,119,207                                                  FFE 1368
  119 CALLDIFV(X(1,2),X(1,1),V1)                                         FFE 1369
      CALLDIFV(X(1,3),X(1,1),V2)                                         FFE 1370
      CALLDIFV(X(1,5),X(1,4),V3)                                         FFE 1371
      CALLDIFV(X(1,6),X(1,4),V4)                                         FFE 1372
      CALLNORM(V1,V2,V5)                                                 FFE 1373
      CALLNORM(V3,V4,V6)                                                 FFE 1374
      FX#ARCCOS(COSVV(V5,V6))                                            FFE 1375
  207 RETURN                                                             FFE 1376
      END(0,1,0,0,0)                                                     FFE 1377
*TYPE(FORTRAN)                                                           FFE 1378
C     OUTPUT DESCRIPTION 3                                               FFE 1379
      SUBROUTINE OUT3                                                    FFE 1380
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE    FFE 1381
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP   FFE 1382
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2  FFE 1383
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)       FFE 1384
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1385
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                          FFE 1386
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,13)                                FFE 1387
  107 FORMAT(12H0          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)/12HFFE 1388
     1          (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H))              FFE 1389
      RETURN                                                             FFE 1390
      END(0,1,0,0,0)                                                     FFE 1391
*TYPE(FORTRAN)                                                           FFE 1392
C     HEADING 4                                                          FFE 1393
      SUBROUTINE HED4                                                    FFE 1394
      WRITEOUTPUTTAPE9,107                                               FFE 1395
  107 FORMAT(45H0DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES)           FFE 1396
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      RETURN                                                                FFE 1397
      END(0,1,0,0,0)                                                        FFE 1398
*TYPE(FORTRAN)                                                              FFE 1399
C     PRELIMINARY SUBROUTINE 4                                              FFE 1400
      SUBROUTINE PRE4                                                       FFE 1401
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE       FFE 1402
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP      FFE 1403
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2     FFE 1404
      )IMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)          FFE 1405
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1406
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                             FFE 1407
      DO107I#2,8,2                                                          FFE 1408
  107 CALLSETKX(IN(I))                                                      FFE 1409
      RETURN                                                                FFE 1410
      END(0,1,0,0,0)                                                        FFE 1411
*TYPE(FORTRAN)                                                              FFE 1412
C     DIFFERENCE BETWEEN BOND DISTANCES                                     FFE 1413
      SUBROUTINE FUN4                                                       FFE 1414
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE       FFE 1415
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP      FFE 1416
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2     FFE 1417
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)          FFE 1418
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1419
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                             FFE 1420
      FX#FUNB(IN(2))-FUNB(IN(6))                                            FFE 1421
      RETURN                                                                FFE 1422
      END(0,1,0,0,0)                                                        FFE 1423
*TYPE(FORTRAN)                                                              FFE 1424
C     OUTPUT DESCRIPTION 4                                                  FFE 1425
      SUBROUTINE OUT4                                                       FFE 1426
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE       FFE 1427
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP      FFE 1428
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2     FFE 1429
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)          FFE 1430
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1431
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                             FFE 1432
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,9)                                    FFE 1433
  107 FORMAT(12H0           (I2,1H,I3,3H) (I2,1H,I3,1H)/12H           (12FFE 1434
     1,1H,I3,3H) (I2,1H,I3,1H))                                             FFE 1435
      RETURN                                                                FFE 1436
      END(0,1,0,0,0)                                                        FFE 1437
*TYPE(FORTRAN)                                                              FFE 1438
C     HEADING 5                                                             FFE 1439
      SUBROUTINE HED5                                                       FFE 1440
      WRITEOUTPUTTAPE9,107                                                  FFE 1441
  107 FORMAT(35HDIFFERENCE BETWEEN TWO BOND ANGLES)                         FFE 1442
      RETURN                                                                FFE 1443
      END(0,1,0,0,0)                                                        FFE 1444
*TYPE(FORTRAN)                                                              FFE 1445
C     DIFFERENCE BETWEEN BOND ANGLES                                        FFE 1446
      SUBROUTINE FUN5                                                       FFE 1447
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE       FFE 1448
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP      FFE 1449
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2     FFE 1450
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)          FFE 1451
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1452
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                             FFE 1453
      FX#FUNA(IN(8))-FUNA(IN(2))                                            FFE 1454
      RETURN                                                                FFE 1455
      END(0,1,0,0,0)                                                        FFE 1456
*TYPE(FORTRAN)                                                              FFE 1457
C     HEADING 6                                                             FFE 1458
      SUBROUTINE HED6                                                       FFE 1459
      WRITEOUTPUTTAPE9,107                                                  FFE 1460
  107 FORMAT(27H0SUM OF SEVERAL BOND ANGLES)                                FFE 1461
      RETURN                                                                FFE 1462
      END(0,1,0,0,0)                                                        FFE 1463
*TYPE(FORTRAN)                                                              FFE 1464
C     PRELIMINARY SUBROUTINE 6                                              FFE 1465
      SUBROUTINE PRE6                                                       FFE 1466
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      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1467
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1468
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1469
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1470
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1471
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1472
      J#IN(2)*6+1                                                       FFE 1473
      DO109I#3,J,2                                                      FFE 1474
  109 CALLSETKX(IN(I))                                                  FFE 1475
      RETURN                                                            FFE 1476
      END(0,1,0,0,0)                                                    FFE 1477
*TYPE(FORTRAN)                                                          FFE 1478
C     SUM OF BOND ANGLES                                                FFE 1479
      SUBROUTINE FUN6                                                   FFE 1480
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1481
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1482
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1483
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1484
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1485
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1486
      N#IN(2)                                                           FFE 1487
      FX#0.0                                                            FFE 1488
      DO111J#1,N                                                        FFE 1489
  111 FX#FX+FUNA(IN(6*J-3))                                             FFE 1490
      RETURN                                                            FFE 1491
      END(0,1,0,0,3)                                                    FFE 1492
*TYPE(FORTRAN)                                                          FFE 1493
C     OUTPUT DESCRIPTION 6                                              FFE 1494
      SUBROUTINE OUT6                                                   FFE 1495
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1496
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1497
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1498
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1499
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1500
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1501
      J#IN(2)*6+2                                                       FFE 1502
      WRITEOUTPUTTAPE9,109,(IN(I),I#3,J)                                FFE 1503
  109 FORMAT(12H0           (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)/(12FFE 1504
     1H            (I2,1H,I3,3H) (I2,1H,I3,3H) (I2,1H,I3,1H)))        FFE 1505
      RETURN                                                            FFE 1506
      END(0,1,0,0,0)                                                    FFE 1507
*TYPE(FORTRAN)                                                          FFE 1508
C     SET UP MATRIX AND GET EIGENVALUE                                  FFE 1509
      SUBROUTINE FUNB(W,Z,ZI)                                           FFE 1510
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1511
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1512
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1513
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1514
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1515
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1516
      DIMENSIONB(3,3),W(3,3),Y(3)                                       FFE 1517
      CALLSTOAA                                                         FFE 1518
      CALLBETA(IN(2),B)                                                 FFE 1519
      IF(NG)123,113,123                                                 FFE 1520
  113 CALLMM(B,AA,W)                                                    FFE 1521
      CALLEIGVAL(W,Y)                                                   FFE 1522
      I#IN(4)                                                           FFE 1523
      Z#Y(I)                                                            FFE 1524
      ZI#SQRTF(Z*0.05066059818)                                         FFE 1525
  123 RETURN                                                            FFE 1526
      END(0,1,0,0,0)                                                    FFE 1527
*TYPE(FORTRAN)                                                          FFE 1528
C     COS ANGLE OF PRINCIPAL AXIS AND VECTOR                            FFE 1529
      SUBROUTINE FUNC(C,Z)                                              FFE 1530
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1531
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1532
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1533
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1534
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1535
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1536
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      DIMENSIONW(3,3),X1(3),X2(3),V1(3),V2(3)                          FFE 1537
      CALLFUNB(W,Y,Z)                                                  FFE 1538
      IF(NG)125,111,125                                                FFE 1539
  111 CALLEIGVEC(W,Y,V1)                                               FFE 1540
      IF(NG)125,115,125                                                FFE 1541
  115 CALLATOM(IN(5),X1)                                               FFE 1542
      CALLATOM(IN(7),X2)                                               FFE 1543
      IF(NG)125,121,125                                                FFE 1544
  121 CALLDIFV(X2,X1,V2)                                               FFE 1545
      C#COSVV(V1,V2)                                                   FFE 1546
  125 RETURN                                                           FFE 1547
      END(0,1,0,0,0)                                                   FFE 1548
*TYPE(FORTRAN)                                                         FFE 1549
C     COS ANGLE OF PRINCIPAL AND CARTESIAN AXES                        FFE 1550
      SUBROUTINE FUNX(C,Z)                                             FFE 1551
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE  FFE 1552
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP FFE 1553
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1554
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)     FFE 1555
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1556
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                        FFE 1557
      DIMENSIONW(3,3),V(3),X(3,4),V1(3),V2(3),AX(3,3)                  FFE 1558
      CALLFUNB(W,Y,Z)                                                  FFE 1559
      CALLSTOBB                                                        FFE 1560
      IF(NG)207,113,207                                                FFE 1561
  113 CALLEIGVEC(W,Y,V)                                                FFE 1562
      IF(NG)207,117,207                                                FFE 1563
  117 DO119I#1,4                                                       FFE 1564
  119 CALLATOM(IN(2*I+4),X(1,I))                                       FFE 1565
      IF(NG)207,123,207                                                FFE 1566
  123 CALLDIFV(X(1,2),X(1,1),V1)                                       FFE 1567
      CALLDIFV(X(1,4),X(1,3),V2)                                       FFE 1568
      CALLAXES(V1,V2,AX)                                               FFE 1569
      I#IN(5)                                                          FFE 1570
      C#COSVV(V,AX(1,I))                                               FFE 1571
  207 RETURN                                                           FFE 1572
      END(0,1,0,0,0)                                                   FFE 1573
*TYPE(FORTRAN)                                                         FFE 1574
C     HEADING 7                                                        FFE 1575
      SUBROUTINE HED7                                                  FFE 1576
      WRITEOUTPUTTAPE9,107                                             FFE 1577
  107 FORMAT(72HRMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL AFFE 1578
     1XIS R. ANGSTROMS/25H0            ATOM       R)                  FFE 1579
      RETURN                                                           FFE 1580
      END(0,1,0,0,0)                                                   FFE 1581
*TYPE(FORTRAN)                                                         FFE 1582
C     PRELIMINARY SUBROUTINE 7                                         FFE 1583
      SUBROUTINE PRE7                                                  FFE 1584
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE  FFE 1585
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP FFE 1586
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1587
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)     FFE 1588
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1589
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                        FFE 1590
      CALLSETKB(IN(2))                                                 FFE 1591
      RETURN                                                           FFE 1592
      END(0,1,0,0,0)                                                   FFE 1593
*TYPE(FORTRAN)                                                         FFE 1594
C     RMS PRINCIPAL DISPLACEMENT                                       FFE 1595
      SUBROUTINE FUN7                                                  FFE 1596
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE  FFE 1597
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP FFE 1598
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1599
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)     FFE 1600
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1601
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                        FFE 1602
      DIMENSIONW(3,3)                                                  FFE 1603
      CALLFUNB(W,Z,FX)                                                 FFE 1604
      RETURN                                                           FFE 1605
      END(0,1,0,0,0)                                                   FFE 1606
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*TYPE(FORTRAN)                                                                  FFE 1607
C       OUTPUT DESCRIPTION 7                                                    FFE 1608
        SUBROUTINE OUT7                                                         FFE 1609
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE         FFE 1610
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP        FFE 1611
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2       FFE 1612
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)            FFE 1613
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)      FFE 1614
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)                               FFE 1615
        WRITEOUTPUTTAPE9,107,(IN(I),I#2,4)                                      FFE 1616
  107 FORMAT(12HO          (12,1H,I3,6H)      I1)                             FFE 1617
        RETURN                                                                  FFE 1618
        END(0,1,0,0,0)                                                          FFE 1619
*TYPE(FORTRAN)                                                                  FFE 1620
C       HEADING 8                                                               FFE 1621
        SUBROUTINE HED8                                                         FFE 1622
        WRITEOUTPUTTAPE9,107                                                    FFE 1623
  107 FORMAT(63HOANGLE BETWEEN PRINCIPAL AXIS R AND VECTOR DEFINED BY TWFFE 1624
     1O ATOMS/40HO          ATOM       R          VECTOR)                      FFE 1625
        RETURN                                                                  FFE 1626
        END(0,1,0,0,0)                                                          FFE 1627
*TYPE(FORTRAN)                                                                  FFE 1628
C       PRELIMINARY SUBROUTINE 8                                                FFE 1629
        SUBROUTINE PRE8                                                         FFE 1630
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE         FFE 1631
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP        FFE 1632
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2       FFE 1633
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)            FFE 1634
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)      FFE 1635
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)                               FFE 1636
        CALLSETKB(IN(2))                                                        FFE 1637
        DO109I#5,7,2                                                            FFE 1638
  109   CALLSETKX(IN(I))                                                        FFE 1639
        RETURN                                                                  FFE 1640
        END(0,1,0,0,0)                                                          FFE 1641
*TYPE(FORTRAN)                                                                  FFE 1642
C       ANGLE BETWEEN PRINCIPAL AXIS AND VECTOR                                 FFE 1643
        SUBROUTINE FUN8                                                         FFE 1644
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE         FFE 1645
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP        FFE 1646
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2       FFE 1647
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)            FFE 1648
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)      FFE 1649
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)                               FFE 1650
        CALLFUNC(C,Z)                                                           FFE 1651
        FX#ARCCOS(C)                                                            FFE 1652
        RETURN                                                                  FFE 1653
        END(0,1,0,0,0)                                                          FFE 1654
*TYPE(FORTRAN)                                                                  FFE 1655
C       OUTPUT DESCRIPTION 8                                                    FFE 1656
        SUBROUTINE OUT8                                                         FFE 1657
        COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE         FFE 1658
        COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,E1,E,IH,NSP        FFE 1659
        COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2       FFE 1660
        DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)            FFE 1661
        DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)      FFE 1662
        DIMENSION P(300),ROW(6),KI1(300),KI2(300)                               FFE 1663
        WRITEOUTPUTTAPE9,107,(IN(I),I#2,8)                                      FFE 1664
  107 FORMAT(12HO          (12,1H,I3,6H)      I1,5H     (12,1H,I3,3H) (12,FFE 1665
     1H,I3,1H))                                                                 FFE 1666
        RETURN                                                                  FFE 1667
        END(0,1,0,0,0)                                                          FFE 1668
*TYPE(FORTRAN)                                                                  FFE 1669
C       HEADING 9                                                               FFE 1670
        SUBROUTINE HED9                                                         FFE 1671
        WRITEOUTPUTTAPE9,107                                                    FFE 1672
  107 FORMAT(113HORMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL FFE 1673
     1AXIS R PROJECTED ON VECTOR DEFINED BY TWO ATOMS. ANGSTROMS/40HO   FFE 1674
     2          ATOM       R          VECTOR)                              FFE 1675
        RETURN                                                                  FFE 1676
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      END(0,1,0,0,0)                                                    FFE 1677
*TYPE(FORTRAN)                                                          FFE 1678
C     PRINCIPAL AXIS PROJECTED ON VECTOR,                               FFE 1679
      SUBROUTINE FUN9                                                   FFE 1680
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1681
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1682
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1683
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1684
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1685
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1686
      CALLFUNC(C,Z)                                                     FFE 1687
      FX#C*Z                                                            FFE 1688
      RETURN                                                            FFE 1689
      END(0,1,0,0,0)                                                    FFE 1690
*TYPE(FORTRAN)                                                          FFE 1691
C     HEADING 10                                                        FFE 1692
      SUBROUTINE HED10                                                  FFE 1693
      WRITEOUTPUTTAPE9,107                                              FFE 1694
  107 FORMAT(85H0ANGLE BETWEEN PRINCIPAL AXIS R AND AXIS I OF CARTESIAN FFE 1695
     1SYSTEM DEFINED BY TWO VECTORS/45H0                ATOM     R  I   DEFIFFE 1696
     2NING VECTORS)                                                     FFE 1697
      RETURN                                                            FFE 1698
      END(0,1,0,0,0)                                                    FFE 1699
*TYPE(FORTRAN)                                                          FFE 1700
C     PRELIMINARY SUBROUTINE 10                                         FFE 1701
      SUBROUTINE PRE10                                                  FFE 1702
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1703
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1704
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1705
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1706
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1707
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1708
      CALLSETKB(IN(2))                                                  FFE 1709
      DO109I#6,12,2                                                     FFE 1710
  109 CALLSETKX(IN(I))                                                  FFE 1711
      RETURN                                                            FFE 1712
      END(0,1,0,0,0)                                                    FFE 1713
*TYPE(FORTRAN)                                                          FFE 1714
C     ANGLE BETWEEN PRINCIPAL AND CARTESIAN AXES                        FFE 1715
      SUBROUTINE FUN10                                                  FFE 1716
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1717
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1718
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1719
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1720
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1721
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1722
      CALLFUNX(C,Z)                                                     FFE 1723
      FX#ARCCOS(C)                                                      FFE 1724
      RETURN                                                            FFE 1725
      END(0,1,0,0,0)                                                    FFE 1726
*TYPE(FORTRAN)                                                          FFE 1727
C     OUTPUT DESCRIPTION 10                                             FFE 1728
      SUBROUTINE OUT10                                                  FFE 1729
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1730
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1731
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KII,KI2 FFE 1732
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1733
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1734
      DIMENSION P(300),ROW(6),KII(300),KI2(300)                         FFE 1735
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,13)                               FFE 1736
  107 FORMAT(12H0          (I2,1H,I3,4H)   I1,I3,4H   (I2,1H,I3,3H) (I2,FFE 1737
     1 1H,I3,1H)/30H                          (I2,1H,I3,3H) (I2,1H,I3,FFE 1738
     2 1H))                                                             FFE 1739
      RETURN                                                            FFE 1740
      END(0,1,0,0,0)                                                    FFE 1741
*TYPE(FORTRAN)                                                          FFE 1742
C     HEADING 11                                                        FFE 1743
      SUBROUTINE HED11                                                  FFE 1744
      WRITEOUTPUTTAPE9,107                                              FFE 1745
  107 FORMAT(101H0RMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL FFE 1746
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     1AXIS R PROJECTED ON AXIS I OF CARTESIAN SYSTEM/34H DEFINED BY TWO FFE 1747
     2VECTORS. ANGSTROMS/45HO            ATOM     R  I   DEFINING VECTORFFE 1748
     3S)                                                                FFE 1749
      RETURN                                                            FFE 1750
      END(0,1,0,0,0)                                                    FFE 1751
*TYPE(FORTRAN)                                                          FFE 1752
C     PRINCIPAL AXIS PROJECTED ON CARTESIAN AXIS                        FFE 1753
      SUBROUTINE FUN11                                                  FFE 1754
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1755
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1756
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1757
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1758
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1759
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1760
      CALLFUNX(C,Z)                                                     FFE 1761
      FX#C*Z                                                            FFE 1762
      RETURN                                                            FFE 1763
      END(0,1,0,0,0)                                                    FFE 1764
*TYPE(FORTRAN)                                                          FFE 1765
C     MEAN SQUARE RADIAL DISPLACEMENT                                   FFE 1766
      SUBROUTINE FUNR(I,RSQ)                                            FFE 1767
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1768
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1769
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1770
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1771
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1772
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1773
      DIMENSIONB(3,3),BAA(3,3)                                          FFE 1774
      CALLSTOAA                                                         FFE 1775
      CALLBETA(I,B)                                                     FFE 1776
      CALLMM(B,AA,BAA)                                                  FFE 1777
      RSQ#TRACE(BAA)*0.0506605918                                       FFE 1778
      RETURN                                                            FFE 1779
      END(0,1,0,0,0)                                                    FFE 1780
*TYPE(FORTRAN)                                                          FFE 1781
C     COMPUTE QUANTITIES FOR MEAN BOND DISTANCE                         FFE 1782
      SUBROUTINE FUNCR(C,R)                                             FFE 1783
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1784
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1785
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1786
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1787
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1788
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1789
      DIMENSIONC(2),X(3,2),V(3)                                         FFE 1790
      DO115I#1,2                                                        FFE 1791
      CALLFUNR(IN(2*I),RSQ)                                             FFE 1792
      CALLFUNXI(IN(2*I),IN(2),XISQ)                                     FFE 1793
      C(I)#RSQ-XISQ                                                     FFE 1794
  115 CALLATOM(IN(2*I),X(1,I))                                          FFE 1795
      CALLDIFV(X(1,2),X(1,1),V)                                         FFE 1796
      R#SQRTF(VMV(V,AA,V))                                              FFE 1797
      RETURN                                                            FFE 1798
      END(0,1,0,0,0)                                                    FFE 1799
*TYPE(FORTRAN)                                                          FFE 1800
C     MEAN SQUARE DISPLACEMENT IN GIVEN DIRECTION                       FFE 1801
      SUBROUTINE FUNXI(I,J,XISQ)                                        FFE 1802
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1803
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1804
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1805
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1806
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1807
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1808
      DIMENSIONI(2),J(4),B(3,3),X1(3),X2(3),V(3),BAA(3,3),AABAA(3,3)    FFE 1809
      CALLSTOAA                                                         FFE 1810
      CALLBETA(I,B)                                                     FFE 1811
      CALLATOM(J,X1)                                                    FFE 1812
      CALLATOM(J(3),X2)                                                 FFE 1813
      IF(NG)207,117,207                                                 FFE 1814
  117 CALLDIFV(X2,X1,V)                                                 FFE 1815
      D#VMV(V,AA,V)                                                     FFE 1816
```

```
      IF(D)123,123,201                                                    FFE 1817
  123 NG#10                                                               FFE 1818
      GOTO207                                                             FFE 1819
  201 CALLMM(B,AA,BAA)                                                    FFE 1820
      CALLMM(AA,BAA,AABAA)                                                FFE 1821
      XISQ#VMV(V,AABAA,V)*0.0506605918/D                                  FFE 1822
  207 RETURN                                                              FFE 1823
      END(0,1,0,0,0)                                                      FFE 1824
*TYPE(FORTRAN)                                                            FFE 1825
C     HEADING 12                                                          FFE 1826
      SUBROUTINE HED12                                                    FFE 1827
      WRITEOUTPUTTAPE9,107                                                FFE 1828
  107 FORMAT(83HORMS COMPONENT OF THERMAL DISPLACEMENT IN DIRECTION DEFIFFE 1829
     1NED BY TWO ATOMS. ANGSTROMS/40HO            ATOM                  VFFE 1830
     2ECTOR)                                                              FFE 1831
      RETURN                                                              FFE 1832
      END(0,1,0,0,0)                                                      FFE 1833
*TYPE(FORTRAN)                                                            FFE 1834
C     PRELIMINARY SUBROUTINE 12                                           FFE 1835
      SUBROUTINE PRE12                                                    FFE 1836
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE     FFE 1837
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP    FFE 1838
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2   FFE 1839
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)        FFE 1840
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1841
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                           FFE 1842
      CALLSETKB(IN(2))                                                    FFE 1843
      DO109I#4,6,2                                                        FFE 1844
  109 CALLSETKX(IN(I))                                                    FFE 1845
      RETURN                                                              FFE 1846
      END(0,1,0,0,0)                                                      FFE 1847
*TYPE(FORTRAN)                                                            FFE 1848
C     RMS DISPLACEMENT IN GIVEN DIRECTION                                 FFE 1849
      SUBROUTINE FUN12                                                    FFE 1850
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE     FFE 1851
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP    FFE 1852
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2   FFE 1853
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)        FFE 1854
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1855
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                           FFE 1856
      CALLFUNXI(IN(2),IN(4),XISQ)                                         FFE 1857
      FX#SQRTF(XISQ)                                                      FFE 1858
      RETURN                                                              FFE 1859
      END(0,1,0,0,0)                                                      FFE 1860
*TYPE(FORTRAN)                                                            FFE 1861
C     OUTPUT DESCRIPTION 12                                               FFE 1862
      SUBROUTINE OUT12                                                    FFE 1863
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE     FFE 1864
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP    FFE 1865
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2   FFE 1866
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)        FFE 1867
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1868
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                           FFE 1869
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,7)                                  FFE 1870
  107 FORMAT(12HO           (I2,1H,I3,12H)          (I2,1H,I3,3H) (I2,1H,FFE 1871
     1I3,1H))                                                             FFE 1872
      RETURN                                                              FFE 1873
      END(0,1,0,0,0)                                                      FFE 1874
*TYPE(FORTRAN)                                                            FFE 1875
C     HEADING 13                                                          FFE 1876
      SUBROUTINE HED13                                                    FFE 1877
      WRITEOUTPUTTAPE9,107                                                FFE 1878
  107 FORMAT(51HORMS RADIAL THERMAL DISPLACEMENT OF ATOM. ANGSTROMS)      FFE 1879
      RETURN                                                              FFE 1880
      END(0,1,0,0,0)                                                      FFE 1881
*TYPE(FORTRAN)                                                            FFE 1882
C     RMS RADIAL DISPLACEMENT                                             FFE 1883
      SUBROUTINE FUN13                                                    FFE 1884
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE     FFE 1885
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP    FFE 1886
```

```
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1887
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1888
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1889
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1890
      CALLFUNR(IN(2),RSQ)                                               FFE 1891
      FX#SQRTF(RSQ)                                                     FFE 1892
      RETURN                                                            FFE 1893
      END(0,1,0,0,0)                                                    FFE 1894
*TYPE(FORTRAN)                                                          FFE 1895
C     OUTPUT DESCRIPTION 13                                             FFE 1896
      SUBROUTINE OUT13                                                  FFE 1897
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1898
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1899
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1900
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1901
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1902
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1903
      WRITEOUTPUTTAPE9,107,(IN(I),I#2,3)                                FFE 1904
  107 FORMAT(12H0           (12,1H,13,1H))                              FFE 1905
      RETURN                                                            FFE 1906
      END(0,1,0,0,0)                                                    FFE 1907
*TYPE(FORTRAN)                                                          FFE 1908
C     HEADING 14                                                        FFE 1909
      SUBROUTINE HED14                                                  FFE 1910
      WRITEOUTPUTTAPE9,107                                              FFE 1911
  107 FORMAT(88H0INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. SECOFFE 1912
     1ND ATOM ASSUMED TO RIDE ON FIRST)                                 FFE 1913
      RETURN                                                            FFE 1914
      END(0,1,0,0,0)                                                    FFE 1915
*TYPE(FORTRAN)                                                          FFE 1916
C     PRELIMINARY SUBROUTINE 14                                         FFE 1917
      SUBROUTINE PRE14                                                  FFE 1918
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1919
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1920
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1921
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1922
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1923
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1924
      DO109I#2,4,2                                                      FFE 1925
      CALLSETKX(IN(I))                                                  FFE 1926
  109 CALLSETKB(IN(I))                                                  FFE 1927
      RETURN                                                            FFE 1928
      END(0,1,0,0,0)                                                    FFE 1929
*TYPE(FORTRAN)                                                          FFE 1930
C     MEAN BOND DISTANCE ASSUMING RIDING                                FFE 1931
      SUBROUTINE FUN14                                                  FFE 1932
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1933
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1934
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1935
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1936
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1937
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1938
      DIMENSIONC(2)                                                     FFE 1939
      CALLFUNCR(C,R)                                                    FFE 1940
      FX#R+(C(2)-C(1))/(2.0*R)                                          FFE 1941
      RETURN                                                            FFE 1942
      END(0,1,0,0,0)                                                    FFE 1943
*TYPE(FORTRAN)                                                          FFE 1944
C     HEADING 15                                                        FFE 1945
      SUBROUTINE HED15                                                  FFE 1946
      WRITEOUTPUTTAPE9,107                                              FFE 1947
  107 FORMAT(87H0INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. ATOMFFE 1948
     1S ASSUMED TO MOVE INDEPENDENTLY)                                  FFE 1949
      RETURN                                                            FFE 1950
      END(0,1,0,0,0)                                                    FFE 1951
*TYPE(FORTRAN)                                                          FFE 1952
C     MEAN INTERATOMIC DISTANCE ASSUMING INDEPENDENT MOTION             FFE 1953
      SUBROUTINE FUN15                                                  FFE 1954
      COMMON NG,IPM,NP,IAM,NS,NV,JXP,JX,JBP,JB,NM,SCALE,ITF,NQ,INSAVE   FFE 1955
      COMMON DMAX,NA,F,FX,LNZ,KK,KKD,SAVEA,SAVEP,VARA,VARP,EI,E,IH,NSP  FFE 1956
```

```
      COMMON TITLE,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,P,ROW,KI1,KI2 FFE 1957
      DIMENSION TITLE(12),PM(20100),DP(200),DFDP(200),AM(21),DA(6)      FFE 1958
      DIMENSION DFDA(6),IN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3)FFE 1959
      DIMENSION P(300),ROW(6),KI1(300),KI2(300)                         FFE 1960
      DIMENSIONC(2)                                                     FFE 1961
      CALLFUNCR(C,R)                                                    FFE 1962
      FX#R+(C(2)+C(1))/(2.0*R)                                          FFE 1963
      RETURN                                                            FFE 1964
      END(0,1,0,0,0)                                                    FFE 1965
*TYPE(FORTRAN)                                                          FFE 1966
C     DUMMY SUBROUTINE. MAY BE CHANGED BY USER.                         FFE 1967
      SUBROUTINE SETA(A)                                                FFE 1968
      RETURN                                                            FFE 1969
      END(0,1,0,0,0)                                                    FFE 1970
*TYPE(FORTRAN)                                                          FFE 1971
C     DUMMY SUBROUTINE. MAY BE CHANGED BY USER.                         FFE 1972
      SUBROUTINE SETP(P)                                                FFE 1973
      RETURN                                                            FFE 1974
      END(0,1,0,0,0)                                                    FFE 1975
```

SUBROUTINES FOR EXAMPLES

```
*TYPE(FORTRAN)                                                          FFE 1976
C     EXAMPLES 1 AND 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.     FFE 1977
      SUBROUTINE SETA(A)                                                FFE 1978
      DIMENSION A(6)                                                    FFE 1979
      A(2)#A(1)                                                         FFE 1980
      RETURN                                                            FFE 1981
      END(0,1,0,0,0)                                                    FFE 1982
*TYPE(FORTRAN)                                                          FFE 1983
C     EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.            FFE 1984
      SUBROUTINE SETP(P)                                                FFE 1985
      DIMENSION P(100)                                                  FFE 1986
      P(5)#P(4)                                                         FFE 1987
      RETURN                                                            FFE 1988
      END(0,1,0,0,0)                                                    FFE 1989
*TYPE(FORTRAN)                                                          FFE 1990
C     EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.            FFE 1991
      SUBROUTINE SETP(P)                                                FFE 1992
      DIMENSION P(100)                                                  FFE 1993
      P(17)#P(16)                                                       FFE 1994
      P(20)#P(19)                                                       FFE 1995
      P(24)#-P(23)                                                      FFE 1996
      RETURN                                                            FFE 1997
      END(0,1,0,0,0)                                                    FFE 1998
```

DATA FOR EXAMPLES

```
*DATA                                                                   FFE 1999
EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT. FFE 2000
  1  6  1  5  4  3  1  0  0                                            FFE 2001
 .4155727 .2676554 .1179998 .5294765 .5294765 .3333333                 FFE 2002
111100                                                                  FFE 2003
        1.0                                                             FFE 2004
 .85384856-7 .73725640-7-.29955735-7-.68440656-8 .13675298-6-.57040983-7FFE 2005
 .11775529-7 .97987015-7 .20795807-7 .33845897-7                        FFE 2006
    4.913        0    5.404        0        0     -0.5                 FFE 2007
     .005        0     .010        0        0                          FFE 2008
           1-2           -2           -3                              FFE 2009
           2-1           -1     .33333333+3                           FFE 2010
           1              2-1   .33333333-3                           FFE 2011
```

```
              2                  1-2   .6666667+3                                  FFE 2012
              2                  1     .66666667-3                                  FFE 2013
   1  2300   1  2                                                                  FFE 2014
   1  2300   1300                                                                 FFE 2015
   2  1  2   2300   1  3                                                          FFE 2016
   2  1300   2300   1305                                                         FFE 2017
   2  1300   2300   1  2                                                          FFE 2018
   3  2300   1  2   1  3   2300   1300   1305                                     FFE 2019
   4  2300   1  2   2300   1300                                                   FFE 2020
   5  1  2   2300   1  3   1300   2300   1305                                     FFE 2021
   0                                                                             FFE 2022
*DATA                                                                            FFE 2023
EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.         FFE 2024
   1  0  1  5                                                                    FFE 2025
     4.913          0     5.404          0          0      -0.5                  FFE 2026
      .005          0      .010          0          0                           FFE 2027
              1-2              -2                 -3                           FFE 2028
              2-1              -1     .33333333+3                               FFE 2029
              1                 2-1   .33333333-3                               FFE 2030
              2                 1-2   .6666667+3                                FFE 2031
              2                 1     .66666667-3                                FFE 2032
   1  2300   1  2                                                                FFE 2033
   1  2300   1300                                                               FFE 2034
   2  1  2   2300   1  3                                                        FFE 2035
   2  1300   2300   1305                                                       FFE 2036
   2  1300   2300   1  2                                                        FFE 2037
   3  2300   1  2   1  3   2300   1300   1305                                   FFE 2038
   4  2300   1  2   2300   1300                                                 FFE 2039
   5  1  2   2300   1  3   1300   2300   1305                                   FFE 2040
 207  2  0                                                                      FFE 2041
 108  1  2      2300   1  2                                                     FFE 2042
 110  1  2         2300   1  2   2300   1  3                                   FFE 2043
 110  2300         2300   2  0   2300   2700                                   FFE 2044
  12  1  2   2300   1  2                                                        FFE 2045
  12  2300   2300   1  2                                                        FFE 2046
  13  1  2                                                                     FFE 2047
  13  2300                                                                     FFE 2048
  15  2300   1  2                                                              FFE 2049
   0                                                                           FFE 2050


*TYPE(BINARY)                                                                  FFE 2051
```

PROGRAM OUTPUT FOR EXAMPLES

```
EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT.

INPUT DATA TO BE READ FROM CARDS

NUMBER OF STRUCTURE PARAMETERS IS   6

VARIANCE-COVARIANCE MATRIX AND PARAMETER SELECTION INFORMATION WILL
BE USED

NUMBER OF SYMMETRY CARDS IS  5

CELL PARAMETER ERRORS ARE
TO BE READ IN THE FORM OF STANDARD ERRORS

ORDER OF THE VARIANCE-COVARIANCE MATRIX FOR THE STRUCTURE PARAMETERS IS  4

PERIOD OF THE POSITION PARAMETERS IN THE PARAMETER LIST IS  3

POSITION OF THE FIRST X COORDINATE IN THE PARAMETER LIST IS  1

INPUT DATA

  I      P(I)   KII(I)

  1    0.4156     1
  2    0.2677     1
  3    0.1180     1
  4    0.5295     1
  5    0.5295     0
  6    0.3333     0


EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT.

CELL PARAMETERS

     4.9130      0.          5.4040      0.          0.         -0.5000

STANDARD ERRORS, RESPECTIVELY, OF THE ABOVE CELL PARAMETERS

     0.0050      0.          0.0100      0.          0.          0.

SYMMETRY INFORMATION

     TRANSFORMED X           TRANSFORMED Y           TRANSFORMED Z

    -0.       1-2           -0.       -2-0          -0.       -3-0
    -0.       2-1           -0.       -1-0           0.333333 3-0
    -0.      -1-0           -0.        2-1           0.333333-3-0
    -0.      -2-0           -0.        1-2           0.666667 3-0
    -0.       2-0           -0.        1-0           0.666667-3-0


EXAMPLE 1. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES CARD INPUT.

INTERATOMIC DISTANCE IN ANGSTROMS

              ( 2,300) ( 1,  2)
                                        1.6012 +OR- 0.0019 ( 0.0012)

              ( 2,300) ( 1,300)
                                        1.6131 +OR- 0.0021 ( 0.0012)
```

```
BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX

          ( 1,  2) ( 2,300) ( 1,  3)
                                        109.2048 +OR- 0.1013 ( 0.0975)

          ( 1,300) ( 2,300) ( 1,305)
                                        110.1962 +OR- 0.1689 ( 0.1443)

          ( 1,300) ( 2,300) ( 1,  2)
                                        109.9518 +OR- 0.0875 ( 0.0755)

DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOMS

          ( 2,300) ( 1,  2) ( 1,  3)
          ( 2,300) ( 1,300) ( 1,305)
                                         89.1600 +OR- 0.1128 ( 0.0478)

DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES

          ( 2,300) ( 1,  2)
          ( 2,300) ( 1,300)
                                        -0.0119 +OR- 0.0026 ( 0.0022)

DIFFERENCE BETWEEN TWO BOND ANGLES

          ( 1,  2) ( 2,300) ( 1,  3)
          ( 1,300) ( 2,300) ( 1,305)
                                          0.9914 +OR- 0.1787 ( 0.1681)


EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.

INPUT DATA TO BE READ FROM OR FLS TAPE

VARIANCE-COVARIANCE MATRIX AND PARAMETER SELECTION INFORMATION WILL
BE USED

NUMBER OF SYMMETRY CARDS IS  5

CELL PARAMETER ERRORS ARE
TO BE READ IN THE FORM OF STANDARD ERRORS

NUMBER OF STRUCTURE PARAMETERS IS  24

PERIOD OF THE POSITION PARAMETERS IN THE PARAMETER LIST IS 11

POSITION OF THE FIRST X COORDINATE IN THE PARAMETER LIST IS  5

PERIOD OF THE TEMPERATURE FACTOR COEFFICIENTS IN THE PARAMETER LIST IS 11

POSITION OF THE FIRST TEMPERATURE FACTOR COEFFICIENT IN THE PARAMETER LIST IS  8

ORDER OF THE VARIANCE-COVARIANCE MATRIX FOR THE STRUCTURE PARAMETERS IS 15

INPUT DATA

  I      P(I)  KII(I)

  1    1.0004    1
  2    0.        0
  3    1.0000    0
  4    1.0000    0
  5    0.4156    1
  6    0.2677    1
  7    0.1180    1
  8    0.0039    1
  9    0.0045    1
 10    0.0027    1
```

11	0.0020	1
12	0.0000	1
13	0.0002	1
14	2.0000	0
15	0.5000	0
16	0.5295	1
17	0.5295	0
18	0.3333	0
19	0.0067	1
20	0.0067	0
21	0.0040	1
22	0.0034	1
23	0.0002	1
24	-0.0002	0

EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.

CELL PARAMETERS

4.9130	0.	5.4040	0.	0.	-0.5000

STANDARD ERRORS, RESPECTIVELY, OF THE ABOVE CELL PARAMETERS

0.0050	0.	0.0100	0.	0.	0.

SYMMETRY INFORMATION

TRANSFORMED X		TRANSFORMED Y		TRANSFORMED Z	
-0.	1-2	-0.	-2-0	-0.	-3-0
-0.	2-1	-0.	-1-0	0.333333	3-0
-0.	-1-0	-0.	2-1	0.333333	-3-0
-0.	-2-0	-0.	1-2	0.666667	3-0
-0.	2-0	-0.	1-0	0.666667	-3-0

EXAMPLE 2. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ. USES OR FLS TAPE.

INTERATOMIC DISTANCE IN ANGSTROMS

(2,300) (1, 2) 1.6012 +OR- 0.0019 (0.0012)

(2,300) (1,300) 1.6131 +OR- 0.0021 (0.0012)

BOND ANGLE IN DEGREES. CENTRAL ATOM IS VERTEX

(1, 2) (2,300) (1, 3) 109.2048 +OR- 0.1014 (0.0977)

(1,300) (2,300) (1,305) 110.1962 +OR- 0.1688 (0.1441)

(1,300) (2,300) (1, 2) 109.9518 +OR- 0.0875 (0.0756)

DIHEDRAL ANGLE BETWEEN PLANES EACH DEFINED BY THREE ATOMS

(2,300) (1, 2) (1, 3)
(2,300) (1,300) (1,305) 89.1600 +OR- 0.1128 (0.0477)

DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES

(2,300) (1, 2)
(2,300) (1,300) -0.0119 +OR- 0.0026 (0.0022)

DIFFERENCE BETWEEN TWO BOND ANGLES

(1, 2) (2,300) (1, 3)
(1,300) (2,300) (1,305)

0.9914 +OR- 0.1784 (0.1679)

RMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL AXIS R. ANGSTROMS

ATOM	R	
(1, 0)	1	0.0600 +OR- 0.0073 (0.0073)
(1, 0)	2	0.0619 +OR- 0.0050 (0.0050)
(1, 0)	3	0.0668 +OR- 0.0068 (0.0068)
(2, 0)	1	0.0742 +OR- 0.0033 (0.0033)
(2, 0)	2	0.0785 +OR- 0.0033 (0.0033)
(2, 0)	3	0.0798 +OR- 0.0035 (0.0035)

ANGLE BETWEEN PRINCIPAL AXIS R AND VECTOR DEFINED BY TWO ATOMS

ATOM	R	VECTOR	
(1, 2)	1	(2,300) (1, 2)	76.6802 +OR-56.4312 (56.4311)
(1, 2)	2	(2,300) (1, 2)	79.0386 +OR-57.5388 (57.5340)
(1, 2)	3	(2,300) (1, 2)	17.3808 +OR-39.1984 (39.1957)

ANGLE BETWEEN PRINCIPAL AXIS R AND AXIS I OF CARTESIAN SYSTEM DEFINED BY TWO VECTORS

ATOM	R	I	DEFINING VECTORS	
(1, 2)	1	1	(2,300) (1, 2) (2,300) (1, 3)	76.6802 +OR-56.4312 (56.4311)
(1, 2)	1	2	(2,300) (1, 2) (2,300) (1, 3)	77.3633 +OR-51.2667 (51.2667)
(1, 2)	1	3	(2,300) (1, 2) (2,300) (1, 3)	161.4757 +OR-80.2633 (80.2633)
(1, 2)	2	1	(2,300) (1, 2) (2,300) (1, 3)	79.0386 +OR-57.5388 (57.5340)
(1, 2)	2	2	(2,300) (1, 2) (2,300) (1, 3)	164.9587 +OR-32.7963 (32.7957)
(1, 2)	2	3	(2,300) (1, 2) (2,300) (1, 3)	100.1726 +OR-48.7792 (48.7790)

(1, 2) 3 1 (2,300) (1, 2)
(2,300) (1, 3)
17.3808 +OR-39.1984 (39.1957)

(1, 2) 3 2 (2,300) (1, 2)
(2,300) (1, 3)
81.9750 +OR-43.5891 (43.5834)

(1, 2) 3 3 (2,300) (1, 2)
(2,300) (1, 3)
74.6870 +OR-37.9786 (37.9784)

(2,300) 1 1 (2,300) (2, 0)
(2,300) (2,700)
90.0000 +OR- 0. (0.)

(2,300) 1 2 (2,300) (2, 0)
(2,300) (2,700)
45.2094 +OR-24.2878 (24.2720)

(2,300) 1 3 (2,300) (2, 0)
(2,300) (2,700)
44.7906 +OR-24.2879 (24.2721)

(2,300) 2 1 (2,300) (2, 0)
(2,300) (2,700)
179.9815 +OR- 1.4866 (1.3871)

(2,300) 2 2 (2,300) (2, 0)
(2,300) (2,700)
89.9902 +OR- 3.0562 (2.6073)

(2,300) 2 3 (2,300) (2, 0)
(2,300) (2,700)
90.0183 +OR- 5.7403 (4.8985)

(2,300) 3 1 (2,300) (2, 0)
(2,300) (2,700)
90.0000 +OR- 0. (0.)

(2,300) 3 2 (2,300) (2, 0)
(2,300) (2,700)
135.2073 +OR-24.0921 (24.0671)

(2,300) 3 3 (2,300) (2, 0)
(2,300) (2,700)
45.2073 +OR-24.0921 (24.0672)

RMS COMPONENT OF THERMAL DISPLACEMENT IN DIRECTION DEFINED BY TWO ATOMS. ANGSTROMS

ATOM VECTOR

(1, 2) (2,300) (1, 2)
0.0662 +OR- 0.0067 (0.0067)

(2,300) (2,300) (1, 2)
0.0791 +OR- 0.0022 (0.0022)

RMS RADIAL THERMAL DISPLACEMENT OF ATOM. ANGSTROMS

(1, 2)
0.1090 +OR- 0.0036 (0.0036)

(2,300)
0.1343 +OR- 0.0016 (0.0016)

INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. ATOMS ASSUMED TO MOVE INDEPENDENTLY

(2,300) (1, 2)
1.6072 +OR- 0.0019 (0.0012)

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