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A CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM FOR THE IBM 704

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A CRYSTALLOGRAPHIC FUNCTION AND ERROR PROGRAM FOR THE IBM 704

by

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IDENTIFICATION

OR XFE

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GENERAL DESCRIPTION

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

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

MACHINE REQUIREMENTS

Minimum 704 with

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

---

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

MATHEMATICAL METHOD

The functions which the program computes are of the form

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

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

The standard error of f is given by

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

where

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

and

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

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

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

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

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

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

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

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

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

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

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

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

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

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

CONSTRAINTS ON THE PARAMETERS

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

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

Specifications for Fortran II Subroutines

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

Example 1

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

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

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

Example 2

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

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

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

SPECIFICATIONS FOR SUBROUTINES TO COMPUTE NEW TYPES OF FUNCTIONS

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

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

HEDi

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

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

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

PREi

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

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

FUNi

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

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

OUTi

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

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

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

ARITHMETIC SUBPROGRAMS AVAILABLE FOR PROGRAMMING NEW FUNCTIONS

1. CALL SETKX (IN(K))

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

2. CALL SETKB (IN(K))

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

3. CALL STOAA

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

4. CALL STOBB

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

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

DIMENSION Z(3)

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

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

DIMENSION Z(3,3)

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

7. CALL MM (X, Y, Z)

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

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

8. CALL MV (X, Y, Z)

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

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

9. CALL VM (X, Y, Z)

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

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

10. Function VV(X, Y)

DIMENSION X(3), Y(3)

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

11. Function VMV (W, X, Y)

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

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

12. CALL DIFV (X, Y, Z)

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

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

13. CALL SUMV (X, Y, Z)

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

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

14. Function COSVV (X,Y)

DIMENSION X(3), Y(3)

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

15. Function ARCCOS (X)

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

16. CALL NORM (X, Y, Z)

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

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

17. CALL AXES (U, V, X)

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

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

18. CALL EIGVAL (W,Y)

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

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

19. CALL EIGVEC (W,Y,Z)

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

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

20. Function TRACE (X)

DIMENSION X(3,3)

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

ATOM DESIGNATION AND SYMMETRY TRANSFORMATIONS

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

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

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

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

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

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

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

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

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

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

OPERATING PROCEDURE

Card deck

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

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

3. Segment 2 main deck.

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

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

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

Operating instructions

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

DETAILS OF DATA INPUT

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

Variance-covariance matrix, PM, for structure parameters

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

First card. FORMAT (I9, E9.4)

Columns

1-9 N, the order of the matrix.

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

Subsequent cards. FORMAT (8E9.4)

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

Title

FORMAT (72H)

Columns

1 Blank.

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

Control card integers, IC

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

Columns

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

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

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

Control card, cont'd.

Columns

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

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

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

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

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

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

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

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

Atomic parameters, P

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

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

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

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

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

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

Parameter selection cards

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

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

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

Cell parameters, A

These six direct unit cell parameters must always be supplied.

FORMAT (6E9.4)

Columns

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

Cell parameter errors, AM

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

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

FORMAT (6E9.4)

Columns

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

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

FORMAT (8E9.4)

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

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

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

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

Symmetry cards

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

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

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

Columns

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

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

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

13 Hollerith X, Y, Z, or blank.

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

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

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

or

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

.

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

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

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

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

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

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

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

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

DETAILS OF INSTRUCTION INPUT

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

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

Function 1

One interatomic distance.

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

Function 101

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

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

Function 201

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

Columns

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

Function 2

Angle defined by three atoms.

Columns

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

Function 3

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

Columns

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

Function 4

Difference between two interatomic distances.

Columns

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

Function 5

Difference between two angles each defined by three atoms.

Columns

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

Function 6

The sum of several angles each defined by three atoms.

Columns

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

Function 7

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

Columns

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

Function 107

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

Columns

1-3	107
4-9	Atom designation

Function 207

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

Columns

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

Function 8

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

Columns

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

Function 108

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

Columns

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

Function 208

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

Columns

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

Function 9

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

Columns

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

Function 109

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

Columns

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

Function 209

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

Columns

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

Function 10

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

Columns

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

Function 10, cont'd

Columns

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

Function 110

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

Columns

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

Function 210

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

Columns

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

Function 11

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

Columns

1-3	11
4-9	Atom designation 1

Function 11, cont'd

Columns

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

Function 111

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

Columns

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

Function 211

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

Columns

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

Function 12

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

Columns

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

Function 13

The RMS radial thermal displacement of an atom.

Columns

1-3	13
4-9	Atom designation

Function 14

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

Columns

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

Function 15

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

Columns

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

ERROR INDICATORS

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

Stops

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

Error Returns

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

COMMON STORAGE

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

BINARY DECKS SUPPLIED

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

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

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

FUN5	25

HED6	35
PRE6	38
FUN6	41
OUT6	67
	1018

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

FUN9	24

HED10	53
PRE10	32
FUN10	25
OUT10	60
HED11	62

FUN11	24

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

FUN15	36

	792

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

Storage requirements, Segment 2

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

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

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

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

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

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

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

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

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

```
WTB13 BST 0                    CONSTANT
      END 0

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

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

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

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

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

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

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

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

```
        BCD 1HED17                                          SUBG 023
        BCD 1HED16                                          SUBG 024
        BCD 1HED15                                          SUBG 025
        BCD 1HED14                                          SUBG 026
        BCD 1HED13                                          SUBG 027
        BCD 1HED12                                          SUBG 028
        BCD 1HED11                                          SUBG 029
        BCD 1HED10                                          SUBG 030
        BCD 1HED9                                           SUBG 031
        BCD 1HED8                                           SUBG 032
        BCD 1HED7                                           SUBG 033
        BCD 1HED6                                           SUBG 034
        BCD 1HED5                                           SUBG 035
        BCD 1HED4                                           SUBG 036
        BCD 1HED3                                           SUBG 037
        BCD 1HED2                                           SUBG 038
        BCD 1HED1                                           SUBG 039
HED     BSS 0                                               SUBG 040
        BCD 1PRE20                                          SUBG 041
        BCD 1PRE19                                          SUBG 042
        BCD 1PRE18                                          SUBG 043
        BCD 1PRE17                                          SUBG 044
        BCD 1PRE16                                          SUBG 045
        BCD 1PRE14          SAME AS PRE15                   SUBG 046
        BCD 1PRE14                                          SUBG 047
        BCD 1PRE7           SAME AS PRE 13                  SUBG 048
        BCD 1PRE12                                          SUBG 049
        BCD 1PRE10          SAME AS PRE11                   SUBG 050
        BCD 1PRE10                                          SUBG 051
        BCD 1PRE8           SAME AS PRE9                    SUBG 052
        BCD 1PRE8                                           SUBG 053
        BCD 1PRE7                                           SUBG 054
        BCD 1PRE6                                           SUBG 055
        BCD 1PRE3           SAME AS PRE5                    SUBG 056
        BCD 1PRE4                                           SUBG 057
        BCD 1PRE3                                           SUBG 058
        BCD 1PRE2                                           SUBG 059
        BCD 1PRE1                                           SUBG 060
PRE     BSS 0                                               SUBG 061
```

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

CSETKB   1471 WRB SET KEY WORDS FOR ATOM BETAS                           SETKB1
      SUBROUTINESETKB(I)                                                 SETKB1
C     I=IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER        SETKB1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM   01
```

```
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONK3(3)                                                     SETKB1
      IF(I)123,123,111                                                   SETKB1
  111 K3(1)=6                                                            SETKB1
      J=IC(10)+IC(9)*(I-1)                                               SETKB1
      K=J/36                                                             SETKB1
      K3(2)=J-36*K                                                       SETKB1
      K3(3)=K+1                                                          SETKB1
      CALLSUB15(K3)                                                      SETKB1
  123 RETURN                                                             SETKB1
      END(0,1,0,0,0)                                                     SETKB1

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

CSTOBB   1471 WRB STORE RECIPROCAL METRIC TENSOR                         STOBB101
      SUBROUTINESTOBB                                                    STOBB103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P          COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONAI(6),CI(6),BBII(3),BBJK(3)                               STOBB105
      DO121I=1,3                                                         STOBB107
      IF(A(I))111,111,115                                                STOBB109
  111 NG=6                                                               STOBB111
```

```
      GOTO225                                                           STOBB113
  115 AI(I)=A(I)                                                        STOBB115
      AI(I+3)=A(I)                                                      STOBB117
      CI(I)=A(I+3)                                                      STOBB119
  121 CI(I+3)=A(I+3)                                                    STOBB121
      X=1.0/(AI(1)*AI(2)*AI(3)*(1.0-CI(1)*CI(1)-CI(2)*CI(2)             STOBB123
     1-CI(3)*CI(3)+2.0*CI(1)*CI(2)*CI(3)))                              STOBB125
      DO205I=1,3                                                        STOBB201
      BBII(I)=X*(1.0-CI(I)*CI(I))*AI(I+1)*AI(I+2)/AI(I)                 STOBB203
  205 BBJK(I)=X*AI(I)*(CI(I+1)*CI(I+2)-CI(I))                           STOBB205
      BB(1,1)=BBII(1)                                                   STOBB207
      BB(1,2)=BBJK(3)                                                   STOBB209
      BB(1,3)=BBJK(2)                                                   STOBB211
      BB(2,1)=BBJK(3)                                                   STOBB213
      BB(2,2)=BBII(2)                                                   STOBB215
      BB(2,3)=BBJK(1)                                                   STOBB217
      BB(3,1)=BBJK(2)                                                   STOBB219
      BB(3,2)=BBJK(1)                                                   STOBB221
      BB(3,3)=BBII(3)                                                   STOBB223
  225 RETURN                                                            STOBB225
      END(0,1,0,0,0)                                                    STOBB227

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

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

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

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

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

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

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

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

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

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

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

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

CSUMV     1471 WRB COMPUTE THE SUM OF TWO VECTORS                       SUMV  101
C                  Z(3)=X(3)+Y(3)                                       SUMV  103
      SUBROUTINESUMV(X,Y,Z)                                             SUMV  105
      DIMENSIONX(3),Y(3),Z(3)                                           SUMV  107
      DO111I=1,3                                                        SUMV  109
```

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

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

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

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

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

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

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

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

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

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

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

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

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

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

COUT1    1471 WRB PUT OUT DESCRIPTION OF INTERATOMIC DISTANCE           OUT1 1
      SUBROUTINEOUT1                                                    OUT1 1
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
```

```
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)     DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)   DIM   03
      WRITEOUTPUTTAPE3,107,(IN(I),I=2,5)                                 OUT1  1
  107 FORMAT(12H+          (I2,1H,I3,3H) (I2,1H,I3,1H))                  OUT1  1
      RETURN                                                             OUT1  1
      END(0,1,0,0,0)                                                     OUT1  1

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

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

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

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

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

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

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

CFUN3    1471 WRB DIHEDRAL ANGLE SUBROUTINE                             FUN3  01
      SUBROUTINEFUN3                                                    FUN3  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONX(3,6),V1(3),V2(3),V3(3),V4(3),V5(3),V6(3)               FUN3  05
      CALLSTOAA                                                         FUN3  07
      CALLSTOBB                                                         FUN3  09
      IF(NG)207,113,207                                                 FUN3  11
  113 DO115I=1,6                                                        FUN3  13
  115 CALLATOM(IN(2*I),X(1,I))                                          FUN3  15
      IF(NG)207,119,207                                                 FUN3  17
  119 CALLDIFV(X(1,2),X(1,1),V1)                                        FUN3  19
      CALLDIFV(X(1,3),X(1,1),V2)                                        FUN3  21
      CALLDIFV(X(1,5),X(1,4),V3)                                        FUN3  23
      CALLDIFV(X(1,6),X(1,4),V4)                                        FUN3  25
      CALLNORM(V1,V2,V5)                                                FUN3  01
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```
      CALLNORM(V3,V4,V6)                                                FUN3  03
      FX=ARCCOS(COSVV(V5,V6))                                           FUN3  05
  207 RETURN                                                            FUN3  07
      END(0,1,0,0,0)                                                    FUN3  09

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

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

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

CFUN4    1471 WRB DIFFERENCE BETWEEN BOND DISTANCES                     FUN4  01
      SUBROUTINEFUN4                                                    FUN4  03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      FX=FUND(IN(2))-FUND(IN(6))                                        FUN4  05
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```
      RETURN                                                            FUN4  07
      END(0,1,0,0,0)                                                    FUN4  09

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

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

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

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

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

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

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

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

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

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

CFUNX    1471 WRB COS ANGLE OF PRINCIPAL AND CARTESIAN AXES             FUNX 101
      SUBROUTINEFUNX(C,Z)                                               FUNX 103
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONW(3,3),V(3),X(3,4),V1(3),V2(3),AX(3,3)                   FUNX 105
      CALLFUNB(W,Y,Z)                                                   FUNX 107
      CALLSTOBB                                                         FUNX 109
      IF(NG)207,113,207                                                 FUNX 111
  113 CALLEIGVEC(W,Y,V)                                                 FUNX 113
```

```
      IF(NG)207,117,207                                                 FUNX 115
  117 DO119I=1,4                                                        FUNX 117
  119 CALLATOM(IN(2*I+4),X(1,I))                                        FUNX 119
      IF(NG)207,123,207                                                 FUNX 121
  123 CALLDIFV(X(1,2),X(1,1),V1)                                        FUNX 123
      CALLDIFV(X(1,4),X(1,3),V2)                                        FUNX 125
      CALLAXES(V1,V2,AX)                                                FUNX 201
      I=IN(5)                                                           FUNX 203
      C=COSVV(V,AX(1,I))                                                FUNX 205
  207 RETURN                                                            FUNX 207
      END(0,1,0,0,0)                                                    FUNX 209

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

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

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

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

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

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

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

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

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

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

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

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

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

CHED11    1471 WRB HEADING 11                                               HED11 01
      SUBROUTINEHED11                                                       HED11 03
      WRITEOUTPUTTAPE3,107                                                  HED11 05
  107 FORMAT(101H0RMS COMPONENT OF THERMAL DISPLACEMENT ALONG PRINCIPAL HED11107
     1AXIS R PROJECTED ON AXIS I OF CARTESIAN SYSTEM/34H DEFINED BY TWO HED11108
     2VECTORS. ANGSTROMS/45H0            ATOM     R  I   DEFINING VECTORHED11109
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     3S)                                                                HED11110
      RETURN                                                            HED11 11
      END(0,1,0,0,0)                                                    HED11 13

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

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

CFUNCR   1471 WRB COMPUTE QUANTITIES FOR MEAN BOND DISTANCE             FUNCR 01
      SUBROUTINEFUNCR(C,R)                                              FUNCR 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONC(2),X(3,2),V(3)                                         FUNCR 05
      DO115I=1,2                                                        FUNCR 07
      CALLFUNR(IN(2*I),RSQ)                                             FUNCR 09
      CALLFUNXI(IN(2*I),IN(2),XISQ)                                     FUNCR 11
      C(I)=RSQ-XISQ                                                     FUNCR 13
  115 CALLATOM(IN(2*I),X(1,I))                                          FUNCR 15
      CALLDIFV(X(1,2),X(1,1),V)                                         FUNCR 17
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      R=SQRTF(VMV(V,AA,V))                                              FUNCR 19
      RETURN                                                            FUNCR 21
      END(0,1,0,0,0)                                                    FUNCR 23

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

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

CPRE12   1471 WRB PRELIMINARY SUBROUTINE 12                             PRE12 01
      SUBROUTINEPRE12                                                   PRE12 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
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      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      CALLSETKB(IN(2))                                                  PRE12 05
      DO109I=4,6,2                                                      PRE12 07
  109 CALLSETKX(IN(I))                                                  PRE12 09
      RETURN                                                            PRE12 11
      END(0,1,0,0,0)                                                    PRE12 13

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

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


CFUN13   1471 WRB RMS RADIAL DISPLACEMENT                               FUN13 01
      SUBROUTINEFUN13                                                   FUN13 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
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      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM    03
      CALLFUNR(IN(2),RSQ)                                               FUN13  05
      FX=SQRTF(RSQ)                                                     FUN13  07
      RETURN                                                            FUN13  09
      END(0,1,0,0,0)                                                    FUN13  11

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

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

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

CFUN14   1471 WRB MEAN BOND DISTANCE ASSUMING RIDING                    FUN14  01
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      SUBROUTINEFUN14                                                   FUN14 03
      COMMONNG,IC,PM,DP,DFDP,AM,DA,DFDA,IN,TS,IS,A,AA,BB,F,FX,P         COM   01
      DIMENSIONIC(10),PM(251),DP(251),DFDP(251),AM(21),DA(6),DFDA(6)    DIM   01
      DIMENSIONIN(231),TS(3,48),IS(2,3,48),A(6),AA(3,3),BB(3,3),P(300)  DIM   03
      DIMENSIONC(2)                                                     FUN14 05
      CALLFUNCR(C,R)                                                    FUN14 07
      FX=R+(C(2)-C(1))/(2.0*R)                                          FUN14 09
      RETURN                                                            FUN14 11
      END(0,1,0,0,0)                                                    FUN14 13

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

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