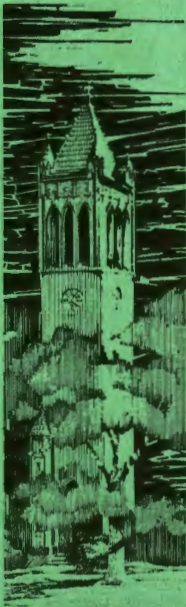


IS-1042



IOWA STATE UNIVERSITY

PACK2, A FORTRAN
CRYSTALLOGRAPHIC MOLECULAR
PACKING PROGRAM

by

Donald E. Williams

AMES LABORATORY

~~PHYSICAL SCIENCES READING ROOM~~

RESEARCH AND

DEVELOPMENT

REPORT

U.S.A.E.C.



IS-1042

Chemistry (UC-4)
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CRYSTALLOGRAPHIC MOLECULAR
PACKING PROGRAM

by

Donald E. Williams

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Ames Laboratory
at
Iowa State University of Science and Technology
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IS-1042

PACK2, A FORTRAN CRYSTALLOGRAPHIC MOLECULAR
PACKING PROGRAM

Donald E. Williams

ABSTRACT

This report describes a computer program which performs an analysis of molecular packing in crystals. All space group symmetries are allowed. The packing energy of a molecular crystal structure, known or proposed, may be evaluated using appropriate nonbonded interatomic potential functions.

For unknown crystal structures, the program may be used to assist the solution of the diffraction phase problem. In this application the program minimizes the packing energy for a molecule of assumed dimensions by a steepest descent method. The adjustable parameters are the molecular translations and rotations, specified internal molecular rotations (subrotations), and the lattice constants.

The program may also be used to study nonbonded interatomic potential functions. These functions can be evaluated by a comparison of the calculated parameters found by the program with the observed parameters for known crystal structures.

INTRODUCTION

The availability of fast digital computers has made possible a more detailed analysis of the packing structure of molecular crystals. Much useful information may be derived from such an analysis. The parameters for nonbonded interatomic potential functions may be checked and improved by analysis of known crystal structures. Thermodynamic quantities for molecular crystals may also be calculated. Examples of such thermodynamic quantities are the heat of sublimation and the energy barrier to molecular rotation in the crystal. Furthermore, the

packing energies and lattice constants for hypothetical structures of different symmetry may be calculated and compared with the known structure.

A second important type of application of packing analysis is to assist in the solution of the diffraction phase problem for unknown crystal structures. If the molecule is of known dimensions, or a reasonable molecular model can be postulated, a possible position of the molecule in the unit cell of known size and symmetry can be found. If the molecule is completely rigid, and is in a general crystallographic position, three rotational and three translational coordinates specify its position. Intramolecular flexibility can be introduced by allowing internal rotation (subrotation) around selected bonds within the molecule. Thus the rotational orientation of a phenyl substituent on a molecule, for example, can be treated as a parameter. The crystal structure found by packing analysis can be quickly checked for rough agreement with diffraction data. The correct packing model can then be refined by means of rigid body structure factor least squares or by the Fourier electron density method.

MATHEMATICAL METHOD

The packing energy of the crystal, E , is defined in the program as the sum of all potential energies of nonbonded atomic interactions. Pairwise additivity of the interatomic potentials is assumed, and zero point energy and rotational energy are neglected. Thus, if the potential energy of interaction between atom \underline{j} in a given molecule and atom \underline{k} in

some surrounding molecule is E_{jk} , then

$$E = \frac{1}{2} \sum E_{jk}$$

where the sum is taken over all of the neighbors of a given molecule.

The nonbonded interatomic potential functions are defined in the subroutine EJKL. In this subroutine, four parameters may be used for each type of interatomic potential. This subroutine may be readily altered by the user; the original program uses the Buckingham formula

$$E_{jk} = -Ad_{jk}^{-6} + B \exp(-d_{jk}/\rho) .$$

For convenience this formula is rewritten as

$$E_{jk} = \left[E_{jk}^0 / (1 - 6\rho/d_{jk}^0) \right] \left[d_{jk}^{-6} d_{jk}^0{}^6 - (6\rho/d_{jk}^0) \exp(d_{jk}^0 - d_{jk})/\rho \right] ,$$

where E_{jk}^0 is the potential energy at the minimum, and d_{jk}^0 is the interatomic distance at the minimum potential. The relations between E_{jk}^0 and d_{jk}^0 and the coefficients of the original equation are

$$E_{jk}^0 = -Ad_{jk}^0{}^{-6} (1 - 6\rho/d_{jk}^0)$$

$$d_{jk}^0{}^7 = (6\rho A/B) \exp(d_{jk}^0/\rho) .$$

INTERATOMIC DISTANCES

We now wish to express the nonbonded distances d_{jk} as a function of the crystal packing structure, with reference to rotation and translation of the molecule in the unit cell, subrotations around bonds within

the molecule, and the lattice constants.

The reference molecule (unit cell fractional coordinates x_j) is surrounded by symmetry related molecules with coordinates x_{kn} , where the first subscript refers to the \underline{k} th atom in the molecule and the second subscript refers to the translation and symmetry operation necessary to obtain the \underline{n} th symmetry related molecule. Thus we have the equation

$$x_{kn} = t_n + s_n x_k,$$

where x_{kn} , t_n , and x_k are column 3-vectors, and s_n is a 3x3 matrix. If we define the 3x3 matrix D which transforms unit cell space into a cartesian reference system, we have in the cartesian system

$$X_{kn} = T_n + S_n X_k,$$

where $X_k = D x_k$, $T_n = D t_n$, and $S_n = D s_n D^{-1}$. The nonbonded inter-atomic distance is

$$d_{jkn} = |X_j - X_{kn}|$$

for the atomic positions of the trial model being considered.

The effect of a small rotation, centered at X_θ^0 , on the reference molecule is given by the equation

$$X_j' = R_\theta (X_j - X_\theta^0) + X_\theta^0, \quad R_\theta = \begin{pmatrix} 1 & -\theta_3 & \theta_2 \\ \theta_3 & 1 & -\theta_1 \\ -\theta_2 & \theta_1 & 1 \end{pmatrix}.$$

The effect of the rotation on a symmetry related atom is given by

$$\mathbf{X}'_{kn} = \mathbf{T}_n + \mathbf{S}_n \left[\mathbf{R}_\theta (\mathbf{X}_k - \mathbf{X}_\theta^0) + \mathbf{X}_\theta^0 \right].$$

The \mathbf{R}_θ matrix is orthonormalized by the program before it is actually used to obtain the new molecular position. The effect of a small translation \mathbf{U} is

$$\mathbf{X}'_j = \mathbf{X}_j + \mathbf{U}, \quad \mathbf{X}'_{kn} = \mathbf{T}_n + \mathbf{S}_n (\mathbf{X}_k + \mathbf{U}).$$

The effect of a small subrotation \mathbf{R}_ψ around a bond in the molecule is given by

$$\mathbf{X}'_j = \mathbf{R}_\psi (\mathbf{X}_j - \mathbf{X}_\psi^0) + \mathbf{X}_\psi^0,$$

where the transformation is applied only to atoms in the rotating group. The center of subrotation, \mathbf{X}_ψ^0 , may be taken as one of the bond atom positions. The matrix \mathbf{R}_ψ may be formed by finding the matrix \mathbf{C} which transforms cartesian space such that the first axis is parallel to the bond direction. We then have

$$\mathbf{R}_\psi = \mathbf{C}^{-1} \mathbf{P} \mathbf{C}, \quad \mathbf{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{pmatrix}.$$

The effect of the subrotation on symmetry related molecules may be found analogously to the θ rotations.

The effect of a small change in the lattice constants is to change the \mathbf{D} matrix to \mathbf{D}' :

$$X_j' = D'D^{-1}X_j, \quad X_{kn}' = D'D^{-1}T_n + D'D^{-1}S_n D(D')^{-1}X_k.$$

STEEPEST DESCENT PROCEDURE

The derivative of E with respect to the parameter p_m is evaluated numerically in the program by incrementing p_m and recalculating E .

Thus

$$\frac{\partial E}{\partial p_m} = \frac{E' - E}{\epsilon_m},$$

where E' is the new value of E found after incrementing the parameter p_m by the amount ϵ_m .

The direction of most rapid change in E is along the gradient vector. To minimize E we move along the gradient by an amount λ to find the parameter shifts Δp_m :

$$\Delta p_m = -\lambda \frac{\partial E}{\partial p_m}.$$

By applying the shifts Δp_m we arrive at a new value of E :

$$E' = E + \sum_m \Delta p_m \frac{\partial E}{\partial p_m} = E - \lambda \sum_m \left(\frac{\partial E}{\partial p_m} \right)^2.$$

Thus the value of λ may be found by estimation of the excess packing energy, $\Delta E = E - E'$, of the current model:

$$\lambda = \Delta E / \sum_m \left(\frac{\partial E}{\partial p_m} \right)^2.$$

The program uses a binary chopping technique to reduce the estimated value of ΔE as the problem converges. A parameter overshoot condition is detected by the program if the current parameter shifts cause the calculated packing energy to increase. When this occurs, ΔE is halved and the problem recycled using half shifts. This process can be repeated several times if necessary.

CLOSE NONBONDED APPROACH TABLE

Since the number of atom pair combinations in a typical unit cell of an organic crystal is quite large, ways must be found to reduce the number of symmetry interactions to be considered. It does not matter that most of these distances can quickly be rejected as too long to be of interest once calculated; we do not wish to calculate the uninteresting distances in the first place.

The number of symmetry-cell translation combinations to be considered can quickly be reduced in the following way. We wish to sum all distances up to $d_{jk}^0 + \Delta d$. If d_{\max}^0 is the maximum d_{jk}^0 in the potential parameter list, a radius $r = (d_{\max}^0 + \Delta d)/2$ about the atoms of the reference molecule needs to be considered. A box with edges parallel to the cartesian axes enclosing the reference molecule with a minimum clearance of r at each face can be constructed. This box may now be symmetry and cell translation transformed. Only those symmetry-cell translation combinations which yield overlapping boxes need to be considered.

A large search still remains, that of sorting through the remaining

symmetry combinations. This can be done on a high speed computer, but preferably not for each steepest descent cycle, because of the time required. We anticipate that the shifts Δp_m will be small, so that a table may be stored in the memory of the computer which gives the atom pairs that are sufficiently close to be considered. This table may be used for several rapid cycles of refinement, until the molecule shifts by a sufficient amount so as to require calculation of a new table. In the original program this table has a maximum of 1800 entries.

MISCELLANEOUS PROGRAM DETAILS

Method of Reference to Potential Functions

Each atom J in the molecule is assigned a reference number IPOTR(J). A reference table IPRET(M, N), where M = IPOTR(J) and N = IPOTR(K), contains an integer IP referencing a set of potential parameters contained in the parameter list.

In summing the interatomic potentials E_{jk} , the program does not apply the factor $\frac{1}{2}$ to the sum, E. Thus each interatomic potential must be multiplied by $\frac{1}{2}$ to put E on an absolute scale. If the interatomic potentials are on an absolute scale, the program calculates and minimizes 2E.

Specification of Symmetry Operations

The program is so arranged that the first symmetry operation must specify the basic molecule, i. e., coordinates x, y, z with no translation. This restriction simplifies the handling of subrotations in making up

the close nonbonded approach table.

Specification of Subrotations

Each atom J in the molecule is assigned a reference number IPSI(J). Intramolecular subrotation interactions are evaluated only for different nonzero values of IPSI(J). In other words, interactions between atoms having the same value of IPSI(J) or if one or both of the atoms has IPSI(J) equal to zero are not considered. Thus the atoms defining the bond about which subrotation occurs will normally be assigned zero IPSI(J) values. A dummy nonzero IPSI(J) value may be assigned to appropriate nonsubrotating group atoms. An example of IPSI(J) assignments is shown in Fig. 1.

Dependent Parameters

User's subroutine PATCH(PARW) is called to set any dependent parameters. This subroutine is called when the parameters are incremented in the derivative section, and again when the steepest descent shifts are obtained. The unselected parameters in the list PARW should be set according to the dependent relationship desired. For example, suppose it is desired that subrotation 2 be equal and opposite in sign to subrotation 1. Then the appropriate Fortran statement in subroutine PATCH is $PARW(14) = -PARW(13)$. The sequence of the parameters in the list PARW is explained in the program Fortran listing.

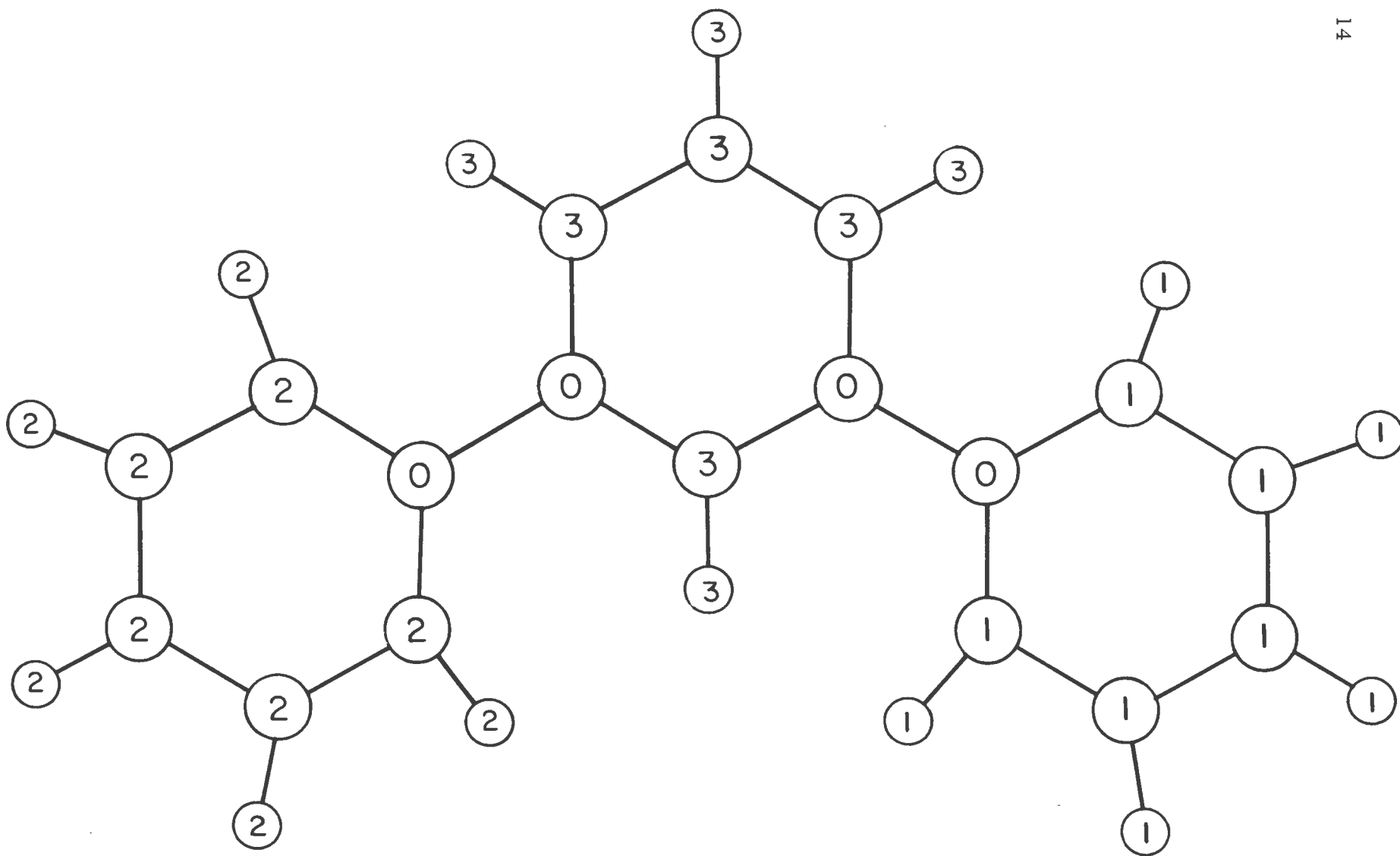


Fig. 1. An example of IPSE(J) assignments for 1,3-diphenylbenzene. Subrotations 1 and 2 may be varied. Dummy subrotation 3 is not varied and serves to include the appropriate intramolecular energy terms in the calculation.

Output Routine

The program normally outputs a list of all input information, information about the makeup of the close nonbonded approach table, and the parameter shifts and packing energy for each steepest descent cycle. The user may alter subroutine OUTPT to output any additional printed information and punched cards desired. This subroutine is called after the NC cycles have been completed. The original routine shown in the Fortran listing outputs the STWE table, a list of distances which are shorter than the distance at the potential minimum by a specified amount, parameter cards for recycling the program, and input cards for a structure factor least squares program. All information in common storage is available to this subroutine.

SYMBOLIC PROGRAM LISTING

START ACCNTACCIS @D.WILLIAMS@ PCGG
 CCMPIL RUN FORTRAN LIST PCGG
 PACK2 CRYSTALLOGRAPHIC PACKING PROGRAM D.WILLIAMS AUG.1964

C
 C
 C INPUT TO PROGRAM

C
 C 1. TAPE ASSIGNMENT CARD FORMAT(7(8X,I2))
 C COL. 9-10 NINP INPUT TAPE NO.
 C COL.19-20 NOUT OUTPUT TAPE NO.
 C COL.29-30 KEY +1 TO TERMINATE PROGRAM, OR BLANK

C
 C 2. TITLE CARD FORMAT(14A5,A2)
 C COL. 1-72 TITLE

C
 C 3. CONTROL CARD FORMAT (8I5,F10.4)
 C COL. 1- 5 NS NUMBER OF SYMMETRY CARDS
 C COL. 6-10 NA NUMBER OF ATOMS IN ASYMMETRIC UNIT
 C COL.11-15 NTHE NUMBER OF RIGID BODIES
 C COL.16-20 NPSI NUMBER OF SUBROTATIONS (ZERO OK)
 C COL.21-25 NPOT NO. SETS OF POTENTIAL PARAMETERS
 C COL.26-30 NPRES WORKING DIMENSION OF IPRES TABLE
 C COL.31-35 INCEL +1 IF CELL TO CARTESIAN TRANSFORM-
 C ATION IS NEEDED, OR BLANK
 C COL.36-40 NC NUMBER OF REFINEMENT CYCLES DESIRED
 C COL.41-50 DELTE ESTIMATE OF E(MODEL)-E(FINAL)

C
 C 4. INITIAL ROTATION MATRIX FORMAT(9F8.2)
 C COL. 1- 8 RMINP(1,1,1) RIGID BODY 1
 C COL. 9-16 RMINP(1,2,1)
 C ...
 C COL.65-72 RMINP(3,3,1)

C
 C 5. ROTATIONAL CENTER AND INITIAL TRANSLATION CARD FORMAT(6F10.2)
 C COL. 1-10 XZTHE(1,1) RIGID BODY 1
 C ...
 C COL.51-60 XTRAN(3,1)

C
 C 6. INITIAL ROTATION MATRIX FORMAT(9F8.2) FOR RIGID BODY 2
 C READ ONLY IF NTHE=2

C
 C 7. ROTATIONAL CENTER AND INITIAL TRANSLATION CARD FORMAT(6F10.2)
 C FOR RIGID BODY 2, READ IF NTHE=2

C
 C 8. LATTICE CONSTANT CARD FORMAT(6F10.4)
 C COL. 1-10 A ANGSTROMS
 C ...
 C COL.51-60 GAMMA DEGREES

C
 C 9. POTENTIAL PARAMETER CARDS FORMAT(4F10.5,32X) NO.=NPOT
 C COL. 1-10 EOJK/2.0 KILOCALORIES/MOLE
 C COL.11-20 DOJK ANGSTROMS
 C COL.21-30 RHOJK ANGSTROMS(-1)
 C COL.31-40 MJK EXPONENT

C
 C 10. SYMMETRY CARDS FORMAT(3F10.8,9F4.0,6X) NO.=NS
 C FIRST SYMMETRY CARD SPECIFIES THE BASIC MOLECULE - I.E.,
 C XYZ WITH NO TRANSLATION
 C COL. 1-10 ST(1,J) TRANSLATION SYMMETRY IN X
 C ...
 C COL.31-34 SS(1,1,J) SYMMETRY MATRIX ELEMENT
 C COL.35-38 SS(1,2,J)
 C ...
 C COL.63-66 SS(3,3,J)

C
 C 11. ATOMIC PARAMETER CARDS FORMAT(3F10.8,3I10,12X) NO.=NA
 C COL. 1-10 XC(1,J) EITHER CELL OR CARTESIAN DEPENDING
 C COL.11-20 XC(2,J) ON INCEL VALUE
 C COL.21-30 XC(3,J)
 C COL.31-40 ITHE(J) RIGID BODY GROUP NUMBER
 C COL.41-50 IPSI(J) SUBROTATION GROUP NUMBER (ZERO OK)

```

C      COL.51-60      IPOTR(J) REFERENCE TO IPRET TABLE
C 12.  SUBROUTINE INFORMATION CARDS  FORMAT(2I10)  NC.=NPSI
C      COL. 1-10     IPSVFC(1,J)   FIRST DEFINING ATOM
C      COL.11-20     IPSVEC(2,J)   SECOND DEFINING ATOM
C 13.  POTENTIAL PARAMETER REFERENCE TABLE  FCRMAT(36I2)
C      COL. 1- 2     IPRET(1,1)
C      COL. 3- 4     IPRET(1,2)
C      ...
C      COL. VARIES   IPRET(NPRET,NPRET)
C 14.  CELL TRANSLATION CARD  FORMAT(6I5,2F10.2)
C      COL. 1- 5     ITCEL(1)  MAXIMUM NEGATIVE A TRANSLATION
C      COL. 6-10     ITCEL(2)  MAXIMUM NEGATIVE B TRANSLATION
C      ...
C      COL.26-30     ITCEL(6)  MAXIMUM POSITIVE C TRANSLATION
C      COL.31-40     RMAX      MAXIMUM DCJK IN POTENTIAL PARAMETERS
C      COL.41-50     DMAX TO BE ADDED TO DCJK TO DETERMINE SUMMATION
C                      LIMIT
C 15.  PARAMETER CONTROL CARDS  FORMAT(72I1)
C      COL. 1       ISEL(1)  +1 IF TO BE VARIED, OR BLANK
C      ...
C      COL.72       ISEL(72)
C      COL. 1       ISEL(73)
C      ...
C      COL.18       ISEL(90)
C 16.  ANY CARDS READ BY SUBROUTINE OUTPT
C
C 17.  STOPPER CARD (CR TAPE ASSIGNMENT CARD FOR NEXT PROBLEM)
C                      FCRMAT(7(8X,12))
C      COL. 1-10     NINP
C      COL.11-20     NOUT
C      COL.21-30     KEY      +1 FOR STOPPER

```

PARAMETERS ARE ORDERED AS FOLLOWS

```

C      I          PAR(I)
C      1- 3      THETA ROTATIONS 1
C      4- 6      TRANSLATIONS 1
C      7- 9      THETA ROTATIONS 2
C      10-12     TRANSLATIONS 2
C      13-24     PSI ROTATIONS
C      25-30     LATTICE CONSTANTS
C      31-34     POTENTIAL PARAMETERS 1
C      35-38     POTENTIAL PARAMETERS 2
C      ...
C      67-70     POTENTIAL PARAMETERS 10
C      71-74     POTENTIAL PARAMETERS 11
C      ...
C      87-90     POTENTIAL PARAMETERS 15

```

GLOSSARY OF SYMBOLS

```

C      A1(I,J)-A3(I,J)  MATRIX WORK CELLS
C      APSI             SUBROUTINE ANGLE
C      C1-C3           CONSTANT WORK CELLS
C      DELTE           ESTIMATE OF E(MODEL)-E(FINAL)
C      DER(I)          DERIVATIVES WITH RESPECT TO THE ITH PARAMETER
C      DINV(I,J)       TRANSFORMS CARTESIAN TO CELL COORDINATES
C      DIST            A DISTANCE
C      DMAT(I,J)       TRANSFORMS CELL TO CARTESIAN COORDINATES
C      CMAX            TO BE ADDED TO DCJK TO DETERMINE SUMMATION LIMIT
C      CSTE(I,J)       EOJK AND DCJK FOR THE JTH ATOM PAIR

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```

C   EZERC      VALUE OF E FOR CURRENT MDEL
C   E          AN ENERGY
C   GRAD2     GRADIENT SQUARED
C   I         INDEX
C   IA        INDEX FOR ATOM 1
C   IARB      INC(X FOR RB 1
C   IB        INDEX FOR ATOM 2
C   IC        CYCLE NUMBER
C   INCEL     CELL TO CARTESIAN TRANSFORMATION INDICATOR
C   IPCTR(I)  REFERENCE TO IPRET TABLE FOR ITH ATOM
C   IPRET(I,J) POTENTIAL PARAMETER NO. FOR TYPE IJ INTERACTION
C   IPSI(I)   SUBROTATION GROUP NUMBER FOR ITH ATOM-IF NCNE, ZERO
C   IPSVEC(I,J) TWO ATOM NUMBERS DEFINING THE JTH SUBROTATION
C   IS        SYMMETRY INDEX
C   ISEL(I)   PARAMETER SELECTION INFORMATION
C   ISWIT     SWITCH CONSTANT FOR GNSYM JTHE ROUTINE
C   ITABW     INDEX FOR JKTAB
C   ITCEL(I)  MIN. AND MAX. CELL TRANSLATIONS TO BE CONSIDERED
C   ITHE(I)   RIGID BODY GROUP NUMBER FOR ITH ATOM
C   ITW(I)    WORKING CELL TRANSLATION
C   IX        INDEX
C   J         INDEX
C   JKTAB(I,J) IA, IB, LTS, AND LSS FOR THE JTH ATOM PAIR
C   JTHE(LTS) VALUE OF LSS CORRESPONDING TO STW(I,LTS)
C   K         INDEX
C   KEY       EXIT CODE
C   KSTOP     SWITCH CONSTANT FOR SHIFT AND DELTE ROUTINE
C   L         INDEX
C   LSS       SYMMETRY MATRIX NUMBER
C   LTS       TRANSLATIONAL SYMMETRY NUMBER
C   LTSM      NUMBER OF TRANSLATIONAL SYMMETRIES CONSIDERED
C   M         INDEX
C   N         INDEX
C   NA        NUMBER OF ATOMS IN RIGID BODY
C   NC        NUMBER OF CYCLES
C   NG        ERROR INDICATOR
C   NINP      INPUT TAPE NUMBER
C   NOUT      OUTPUT TAPE NUMBER
C   NPMAX     MAXIMUM NUMBER OF PARAMETERS
C   NPQT      NUMBER OF SETS OF POTENTIAL PARAMETERS
C   NPRET     WORKING DIMENSION OF IPRET TABLE
C   NPSI      NUMBER OF SUBROTATIONS
C   NS        NUMBER OF SYMMETRY CARDS
C   NTHE      NUMBER OF RIGID BODY GROUPS
C   PAR(I)    REFERENCE PARAMETER LIST
C   PARW(I)   WORKING PARAMETER LIST
C   PINC(I)   PARAMETER INCREMENTS
C   PSINC(I,J) SUBROTATION INCREMENT MATRIX
C   RMAX      LARGEST DOJK IN POTENTIAL PARAMETER LIST
C   RMINC(I,J,K) CRTHCNORMALIZED ROTATION INCREMENT MATRIX FOR RB K
C   RMINP(I,J,K) INITIAL ROTATION MATRIX FOR RIGID BODY K
C   RTPSI(I,J,K) SUBROTATION MATRIX K
C   SHIFT     SHIFT FACTOR
C   SS(I,J,K) SYMMETRY TRANSFORMATION MATRIX FOR KTH OPERATION
C   ST(I,J)   TRANSLATIONAL SYMMETRY VECTOR FOR JTH OPERATION
C   STW(I,LTS) TRANSLATIONAL SYMMETRY INCLUDING CELL TRANSLATIONS
C   TITLE(I)  TITLE
C   V1(I)-V5(I) VECTOR WORK CELLS
C   XC(I,J)   COORDINATES OF JTH ATOM
C   XMAX(I)   MAXIMUM PARAMETERS CONSIDERED BY GNSYM
C   XMIN(I)   MINIMUM PARAMETERS CONSIDERED BY GNSYM
C   XTRAN(I)  INITIAL TRANSLATION

```

```

C      XV(I)          UNIT X VECTOR USED IN RIPSJ
C      XZPSI(I,J)    CENTER OF JTH SUBRGTATION
C      XZTHE(I,K)    CENTER OF ROTATION OF RIGID BDDY K
C      YV(I)          UNIT Y VECTOR USED IN RIPSJ
C
      DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
1  SS(3,3,24), XC(3,100), IPSI(100), IPCTR(100), IPSVEC(2,12),
2  PARW(90), IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
3  V2(3), V3(3), V4(3), V5(3), A1(3,3), A2(3,3), A3(3,3), XTRAN(3,2),
4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200), ISEL(90),
5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
COMMON NINP, NCUT, TITLE, PAR, RMINP, XZTHE, NS, NA, NPSI, INCEL,
1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPCTR, IPSVEC, PARW, IPRET,
2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
4  ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
5  EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
6  DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
C
      XV(1)=1.0
      XV(2)=0.0
      XV(3)=0.0
      YV(1)=0.0
      YV(2)=1.0
      YV(3)=0.0
697 READ 7, NINP, NOUT, KEY
      7 FORMAT(7(8X,I2))
      IF (KEY) 698,698,699
698 CALL INPUT
      CALL DRMAT(PAR(25),DMAT)
      CALL GINV3(DMAT,DINV,NG)
C      TRANSFORM INPUT TO CARTESIAN COORDINATES IF REQUIRED
      IF (INCEL) 1,1,2
2 DO 3 I=1, NA
      CALL MV(DMAT,XC(1,I),V1)
      CO 3 J=1, 3
3 XC(J,I)=V1(J)
1 CONTINUE
C      INITIAL ROTATION AND TRANSLATION
      DO 4 I=1, NA
      IARB=ITHE(I)
      CALL VS(XC(1,I),XZTHE(1,IARB),V1)
      CALL MV(RMINP(1,1,IARB),V1,V2)
      CALL VA(V2,XZTHE(1,IARB),V1)
-4 CALL VA(V1,XTRAN(1,IARB),XC(1,I))
      CO 6 IARB=1, NTHE
      CALL VA(XZTHE(1,IARB),XTRAN(1,IARB),V1)
      DO 6 I=1, 3
6 XZTHE(I,IARB)=V1(I)
C      SELECT INTERATOMIC VECTORS FOR CONSIDERATION
      CALL GNSYM
C      SET UP INCREMENTS
C      ROTATION IN THETA
      DO 51 I=1, 3
      PINC(I+6)=C.002
51 PINC(I)=0.002
C      TRANSLATION
      DO 52 I=4, 6
      PINC(I+6)=C.003
52 PINC(I)=0.003
C      ROTATION IN PSI

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      DO 53 I=13, 24
53  PINC(I)=0.C02
C   LATTICE CONSTANTS
      DO 54 I=25, 27
54  PINC(I)=0.C1
      DO 55 I=28, 30
55  PINC(I)=0.C08
      DO 56 I=31, NPMAX, 4
C   EJKZERC
      PINC(I)=0.C01
C   CJKZERC
      PINC(I+1)=C.005
C   RHCJK
      PINC(I+2)=C.004
C   MJK
56  PINC(I+3)=C.05
C   PREPARE TO BEGIN NC REFINEMENT CYCLES WITH CURRENT JKTAB AND DSTE
C   SET UP INITIAL PARAMETER LIST WITH ZERCS
      DO 11 I=1, 24
11  PAR(I)=0.C
      IC=0
      IF (NC) 401, 401, 999
999 IC=IC+1
C   INITIALIZE SUBROTATION MATRICES
      APSI=0.002
      IF (NPSI) 43,43,44
44  DO 45 J=1, NPSI
45  CALL RIPS(I,J,APSI)
43  CONTINUE
C   CALCULATE SUMS OF DERIVATIVES
      DO 121 J=1, NPMAX
121 DER(J)=0.0
      DO 222 J=1, NPMAX
      IF (ISEL(J)) 222,222,123
123 DO 151 L=1, NPMAX
151 PARW(L)=PAR(L)
      PARW(J)=PAR(J)+PINC(J)
      CALL PATCH(PARW)
      IF (J-4) 131,125,125
125 IF (J-7) 132,226,226
226 IF (J-10) 131,227,227
227 IF (J-13) 132,126,126
126 IF (J-25) 133,127,127
127 IF (J-31) 134,135,135
C   ROTATION PARAMETER
131 CALL DJKL1(ITABW,JKTAB,XC,PARW,SS,STWE,XZTHE,ITHE,IPRET,IPCTR,E)
      GO TO 122
C   TRANSLATION PARAMETER
132 CALL DJKL2(ITABW,JKTAB,XC,PARW,SS,STWE,ITHE,IPRET,IPOTR,E)
      GO TO 122
C   SUBROTATION PARAMETER
133 CALL DJKL3(ITABW,JKTAB,XC,PARW,SS,STWE,IPSI,RTPSI,XZPSI,IPRET,
1  IPCTR,J,E)
      GO TO 122
C   LATTICE PARAMETER
134 CALL DJKL4(ITABW,JKTAB,XC,PARW,SS,STWE,CINV,IPRET,IPOTR,E)
      GO TO 122
C   POTENTIAL PARAMETER
135 E=C.0
      DO 145 I=1, ITABW
      CALL EJKL(I,DSTE(2,I),PARW,JKTAB,IPRET,IPOTR,C1)
145 E=E+C1

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122 DER(J)=(E-EZERC)/PINC(J)
222 CONTINUE
C   CALCULATE GRADIENT SQUARED
    GRAD2=C.0
    DO 161 I=1, NPMAX
      IF (ISEL(I)) 161,161,162
162 GRAD2=GRAD2+DER(I)*DER(I)
161 CONTINUE
    SHIFT=DELTE/GRAD2
    DO 165 I=1, NPMAX
      IF (ISEL(I)) 163,163,164
164 PARW(I)=PAR(I)-SHIFT*DER(I)
      GO TO 165
163 PARW(I)=PAR(I)
165 CONTINUE
    CALL PATCH(PARW)
C   ADJUST XC ARRAY FOR NEXT CYCLE
    KSTOP=1
C   OBTAIN ORTHONORMALIZED ROTATION MATRICES
399 DO 301 IARB=1, NTHE
    K=IARB*6-5
    CALL ROTOR(PARW(K),RMINC(1,1,IARB))
    CALL MM(RMINC(1,1,IARB),RMINP(1,1,IARB),A2)
    DO 301 I=1, 3
      DO 301 J=1, 3
301 RMINP(I,J,IARB)=A2(I,J)
    DO 302 I=1, NA
      IARB=ITHE(I)
      CALL MV(RMINC(1,1,IARB),XC(1,I),V1)
      DO 302 J=1, 3
        K=6*IARB-3+J
302 XC(J,I)=V1(J)+PARW(K)
      DO 379 IARB=1, NTHE
        DO 379 J=1, 3
          K=6*IARB-3+J
379 XZTHE(J,IARB)=XZTHE(J,IARB)+PARW(K)
C   ADJUST FOR SUBROTATIONS
    IF (NPSI) 303,303,304
304 DO 305 J=1, NPSI
      CALL RPSI(J,PARW(J+12))
      DO 305 I=1, NA
        IF (J-IPSI(I)) 305,306,305
306 CALL VS(XC(1,I),XZPSI(1,J),V1)
      CALL MV(RTPSI(1,1,J),V1,V2)
      CALL VA(V2,XZPSI(1,J),XC(1,I))
305 CONTINUE
C   ADJUST FOR LATTICE CONSTANTS
303 CALL ORMAT(PARW(25),DMAT)
    CALL MM(DMAT,DINV,A2)
    DO 311 I=1, NA
      CALL MV(A2,XC(1,I),V1)
      DO 311 J=1, 3
311 XC(J,I)=V1(J)
C   ADJUST STWE AND SS FOR NEW LATTICE CONSTANTS
    DO 501 I=1, LTSM
      CALL MV(A2,STWE(1,I),V1)
      DO 501 J=1, 3
501 STWE(J,I)=V1(J)
    CALL GINV3(A2,A1,NC)
    DO 502 I=1, NS
      CALL MM(A2,SS(1,1,I),A3)
502 CALL MM(A3,A1,SS(1,1,I))

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      CALL GINV3(DMAT,DINV,NG)
C     SET UP NEW DSTE TABLE AND CALCULATE NEW EZERC (C1)
      C1=0.0
      DO 312 I=1, ITABW
      IA=JKTAB(1,I)
      IB=JKTAB(2,I)
      LTS=JKTAB(3,I)
      LSS=JKTAB(4,I)
      CALL MV(SS(1,1,LSS),XC(1,IB),V1)
      CALL VA(STWE(1,LTS),V1,V2)
      CALL MAG(V2,XC(1,IA),DSTE(2,I))
      CALL EJKL(I,DSTE(2,I),PARW,JKTAB,IPRET,IPQTR,DSTE(1,I))
      C1=C1+DSTE(1,I)
312  CONTINUE
C     CHECK NEW VALUE OF EZERO
      IF (EZERC-C1) 313,313,314
313  DO 315 I=1, 24
      IF (ISEL(I)) 315,315,316
316  PARW(I)=SHIFT*DER(I)*(2.0**(-KSTCP))
315  CONTINUE
      DO 371 I=25, NPMAX
      IF (ISEL(I)) 371, 371, 372
372  PARW(I)=PARW(I)+SHIFT*DER(I)*(2.0**(-KSTCP))
371  CONTINUE
      CALL PATCH(PARW)
      DELTE=DELTE*0.5
      KSTOP=KSTOP+1
      IF (KSTOP-4) 399, 314, 314
C     END OF CYCLE
314  EZERC=C1
322  FORMAT(1H0 8H CYCLE I2, 8H EZERO=F10.2, 8H DELTE=F10.4,
1 8H GRAD2=F10.2/1H020H PARAMETER SHIFT)
323  FORMAT(1H0I6,F14.5)
      WRITE OUTPUT TAPE NOUT, 322, IC, EZERC, DELTE, GRAD2
      DO 324 I=1, NPMAX
      IF (ISEL(I)) 324,324,325
325  C2=-SHIFT*DER(I)*(2.0**(1-KSTOP))
      WRITE OUTPUT TAPE NOUT, 323, I, C2
324  CONTINUE
      DO 321 I=25, NPMAX
321  PAR(I)=PARW(I)
      IF (IC-NC) 999,401,401
401  CALL OUTPT
      GO TO 697
699  STCP 87
      END
END      ACCNTA0015 @D.WILLIAMS@
START   ACCNTA0015 @D.WILLIAMS@
CCMPLE  RLN  FORTRAN LIST
C     SUBROUTINE GNSYM
      SUBROUTINE GNSYM
      DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
1  SS(3,3,24), XC(3,100), IPSI(100), IPCTR(100), IPSVEC(2,12),
2  PARW(90), IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
3  V2(3), V3(3), V4(3), V5(3), A1(3,3),A2(3,3),A3(3,3), XTRAN(3,2),
4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200), ISEL(90),
5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
      COMMON NINP, NCUT, TITLE, PAR, RMINP, XZTHE, NS, NA, NPSI, INCEL,
1  NPCT, NPRET, DELTE, ST, SS, XC, IPSI, IPCTR, IPSVEC, PARW,IPRET,

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2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
4  ITW, ISWIT, STW, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
5  EZERC, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
6  DER, PINC, GRAC2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
DIMENSION TCELL(3), TSYM(3)
C  CRTHOGCNALIZF SYMMETRY MATRICES
DO 101 I=1, NS
CALL MV(DMAT,ST(1,I),V1)
DO 123 J=1, 3
123 ST(J,I)=V1(J)
CALL MM(SS(1,1,I),DINV,A1)
101 CALL MM(DMAT,A1,SS(1,1,I))
C  FIND MAX AND MIN XC VALUES
C1=0.5*(RMAX+DMAX)
DO 20 IX=1, 3
XMIN(IX)=100000.0
XMAX(IX)=-100000.0
DO 1 IA=1, NA
IF (XC(IX,IA)-XMIN(IX)) 4,5,5
4 XMIN(IX)=XC(IX,IA)
5 IF (XC(IX,IA)-XMAX(IX)) 1,1,6
6 XMAX(IX)=XC(IX,IA)
1 CONTINUE
XMAX(IX)=XMAX(IX)+C1
XMIN(IX)=XMIN(IX)-C1
20 CONTINUE
C  SELECT APPLICABLE CELL TRANSLATIONS
C  FIRST SYMMETRY CARD IS X Y Z , I.E., ASYMMETRIC UNIT
C  INTRAMOLECULAR DISTANCES AND INTER RIGID BODY DISTANCES
JTWE(1)=1
DO 79 J=1, 3
79 STW(J,1)=ST(J,1)
LTS=1
DO 41 I=1, 3
41 ITW(I)=ITCEL(I)
61 DO 75 I=1, 3
75 V2(I)=FLOATF(ITW(I))
CALL MV(DMAT,V2,TCELL)
DO 62 IS=1, NS
C  REJECT INTRAMOLECULAR DISTANCES IN THIS SECTION
IF (IS+XABSF(ITW(1))+XABSF(ITW(2))+XABSF(ITW(3))-1) 62,62,43
43 CALL VA(TCELL,ST(1,IS),TSYM)
CALL MV(SS(1,1,IS),XMAX,V4)
CALL MV(SS(1,1,IS),XMIN,V5)
CALL VA(TSYM,V4,V1)
CALL VA(TSYM,V5,V2)
DO 51 IX=1, 3
IF (XMAX(IX)-V1(IX)) 53, 52, 52
52 IF (V1(IX)-XMIN(IX)) 53, 51, 51
53 IF (XMAX(IX)-V2(IX)) 62, 54, 54
54 IF (V2(IX)-XMIN(IX)) 62, 51, 51
51 CONTINUE
C  INCLUDE TRANSLATION-SYMMETRY COMBINATION IN JTWE TABLE
LTS=LTS+1
DO 57 I=1, 3
57 STW(I,LTS)=TSYM(I)
JTWE(LTS)=IS
62 CONTINUE
DO 60 I=1, 3
IF (ITW(I)-ITCEL(I+3)) 59,60,60
59 ITW(I)=ITW(I)+1

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      GO TO 61
60  ITW(I)=ITCEL(I)
      LTSM=LTS
C    SELECT INDIVIDUAL INTERATOMIC VECTORS FOR JKTAB(JATCM,KATCM,
C      LTS,LSS,ITABW)  DIMENSION(4,1500) CR SO
C    SET UP DSTE TABLE AND CALCULATE EZERO
      EZERO=0.0
      ITABW=0
      DO 71 LTS=1, LTSM
      LSS=JTW(LTS)
      DO 71 IB=1, NA
      CALL MV(SS(1,1,LSS),XC(1,IB),V1)
      CALL VA(STWE(1,LTS),V1,V2)
      K=IPCTR(IB)
      DO 71 IA=1, NA
C    CHECK ITHE AND IPSI EQUALITY WHEN LTS=1
      IF (LTS-1) 91, 92, 91
92  IF (ITHE(IA)-ITHE(IB)) 91, 93, 91
93  IF (IPSI(IA)-IPSI(IB)) 94, 71, 94
94  IF (IPSI(IA)) 71, 71, 95
95  IF (IPSI(IB)) 71, 71, 91
91  CALL VS(V2,XC(1,IA),V1)
      CIST=SQRT(V1(1)*V1(1)+V1(2)*V1(2)+V1(3)*V1(3))
      J=IPOTR(IA)
      L=IPRET(J,K)
      C1=PAR(4*L+28)
      IF (CIST-DMAX-C1) 80,80,71
80  ITABW=ITABW+1
      JKTAB(1,ITABW)=IA
      JKTAB(2,ITABW)=IB
      JKTAB(3,ITABW)=LTS
      JKTAB(4,ITABW)=LSS
      DSTE(2,ITABW)=CIST
      CALL EJKL(ITABW,CIST,PAR, JKTAB,IPRET,IPCTR,DSTE(1,ITABW))
      EZERO=EZERO+DSTE(1,ITABW)
71  CONTINUE
C    OUTPUT GENSYM INFORMATION
      WRITE OUTPUT TAPE NOUT, 85, NS, LTSM,      ITABW, EZERO,
1  (XMIN(I), XMAX(I), I=1, 3)
85  FORMAT (1H0 5H NS=I2,7H LTSM=I2,          8H ITABW=I4,
1  8H EZERC=F8.4,
2  /1H0      8H XMIN1=F7.2,      8H XMAX1=F7.2,
3           8H XMIN2=F7.2,      8H XMAX2=F7.2,
4           8H XMIN3=F7.2,      8H XMAX3=F7.2)
      RETURN
      END

END      ACCNTA0015 @D.WILLIAMS@
START   ACCNTA0015 @D.WILLIAMS@
CCMPLE  RUN FORTRAN LIST
C    SUBROUTINE INPLT
      SUBROUTINE INPLT
      DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
1  SS(3,3,24), XC(3,100), IPSI(100), IPCTR(100), IPSVEC(2,12),
2  PARW(90), IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
3  V2(3), V3(3), V4(3), V5(3), A1(3,3), A2(3,3), A3(3,3), XTRAN(3,2),
4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTW(200), ISEL(90),
5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
      COMMON NINP, NCUT, TITLE, PAR, RMINP, XZTHE, NS, NA, NPSI, INCEL,
1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPCTR, IPSVEC, PARW,IPRET,

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2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
4  ITW, ISWT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
5  EZERC, ISEL, NG, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
6  CER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
2  FORMAT(14A5,A2)
  READ INPUT TAPE NINP, 2, (TITLE(I),I=1,15)
3  FORMAT(1H014A5,A2)
  WRITE OUTPLT TAPE NOUT, 3, (TITLE(I),I=1,15)
41 FORMAT(8I5,F10.4)
  READ INPUT TAPE NINP, 41, NS, NA, NTHE, NPSI, NPOT, NPRET, INCEL,
  1  NC, DELTE
10 FORMAT(1H0 5H NS=12,5H NA=12,7H NTHE=12, 7H NPSI=12,
  1  7H NPOT=12, 8H NPRET=12, 8H INCEL=12, 5H NC=12,
  2  8H DELTE=F10.5)
  WRITE OUTPUT TAPE NOUT, 10, NS, NA, NTHE, NPSI, NPCT, NPRET,
  1  INCEL, NC, DELTE
6  FORMAT(9F8.2)
8  FORMAT(6F10.2)
  DO 51 K=1, NTHE
  READ INPUT TAPE NINP, 6, ((RMINP(I,J,K),J=1,3),I=1,3)
  READ INPUT TAPE NINP, 8, (XZTHE(I,K),I=1,3), (XTRAN(I,K),I=1,3)
7  FORMAT(1H0 7H RMINP11, 9F10.6)
9  FORMAT(1H0 7H XZTHE11, 3F10.2,7H XTRAN11, 3F10.2)
  WRITE OUTPUT TAPE NOUT, 7, K, ((RMINP(I,J,K),J=1,3),I=1,3)
51 WRITE OUTPLT TAPE NOUT, 9, K, (XZTHE(I,K),I=1,3),K,(XTRAN(I,K),
  1  I=1,3)
4  FORMAT(6F10.4)
  READ INPUT TAPE NINP, 4, (PAR(I), I=25, 30)
5  FORMAT(1H0 20H LATTICE CONSTANTS 3F10.4,3F10.2)
  WRITE OUTPUT TAPE NOUT, 5, (PAR(I), I=25,30)
  DO 29 I=28, 30
29 PAR(I)=PAR(I)/57.29578
17 FORMAT(4F10.5,32X)
  NPMAX=4*NPCT+30
  READ INPUT TAPE NINP, 17, (PAR(J), J=31,NPMAX)
18 FORMAT(1H0 24H POTENTIAL PARAMETERS /1H (/1H 4F10.5))
  WRITE OUTPLT TAPE NOUT, 18, (PAR(J), J=31,NPMAX)
11 FORMAT(3F10.8,9F4.0,6X)
  READ INPUT TAPE NINP, 11, ((ST(I,K),I=1,3),((SS(N,J,K),J=1,3),
  1  N=1,3),K=1,NS)
12 FORMAT(1H0 22H SYMMETRY INFORMATION/1H /(1H 3F12.8,9F8.1))
  WRITE OUTPLT TAPE NOUT, 12, ((ST(I,K),I=1,3),((SS(N,J,K),J=1,3),
  1  N=1,3),K=1,NS)
13 FORMAT(3F10.8,3I10,12X)
  READ INPUT TAPE NINP, 13, ((XC(I,K),I=1,3),ITHE(K),IPSI(K),
  1  IPCTR(K),K=1,NA)
14 FORMAT(1H0 20H ATOMIC INFORMATION/16X,7HITHE(I)3X,7HIPSI(I)3X,
  1  8HIPCTR(I) /(1H 3F10.6,4I10))
  WRITE OUTPLT TAPE NOUT, 14, ((XC(I,K),I=1,3),ITHE(K),IPSI(K),
  1  IPCTR(K),K=1,NA)
15 FORMAT(2I10)
  IF (NPSI) 42, 42, 43
43 READ INPUT TAPE NINP, 15, ((IPSVEC(I,J),I=1,2),J=1,NPSI)
16 FORMAT(1H0 50H SUBROTATION INFORMATION IPSVEC(1,J)
  1  3CH IPSVEC(2,J) J
  2  /1H /(1H 26X,I10,I25,I17))
  WRITE OUTPUT TAPE NOUT, 16, ((IPSVEC(I,J),I=1,2),J,J=1,NPSI)
19 FORMAT(36I2)
42 READ INPUT TAPE NINP, 19, ((IPRET(I,J),J=1,NPRET),I=1,NPRET)
20 FORMAT(1H0 10H IPRET 36I2)
  WRITE OUTPUT TAPE NOUT,20,((IPRET(I,J),J=1,NPRET),I=1,NPRET)

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21 FORMAT(6I5,2F10.2)
   READ INPUT TAPE NINP, 21, (ITCEL(I),I=1,6), RMAX, DMAX
22 FORMAT(1HC 1CH ITCEL 6I5, 7H RMAX=F 6.2,7H DMAX=F 6.2)
   WRITE OUTPLT TAPE NCUT, 22, (ITCEL(I),I=1,6), RMAX, DMAX
   READ INPUT TAPE NINP, 31, (ISEL(I), I=1,NPMAX)
31 FORMAT(7Z11)
   WRITE OUTPLT TAPE NOUT, 32, (ISEL(I),I=1,NPMAX)
32 FORMAT(1HO 25H PARAMETERS SELECTED /1HO2X,
1 4(3I1,1X),12I1,1X,6I1,2X,15(4I1,1X))
   RETURN
   END

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END ACCNTA0015 @D.WILLIAMS@ PCCG
START ACCNTA0015 @D.WILLIAMS@ PCCG
CCMPILE RUN FORTRAN LIST PCCG
C SUBROUTINE RIPSI(JJ,APSI)
  SUBRCUTINE RIPSI(JJ,APSI)
  DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
1 SS(3,3,24), XC(3,100), IPSI(100), IPCTR(100), IPSVEC(2,12),
2 PARW(90), IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
3 V2(3), V3(3), V4(3), V5(3), A1(3,3), A2(3,3), A3(3,3), XTRAN(3,2),
4 XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200), ISEL(90),
5 XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
6 JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
  COMMON NINP, NCUT, TITLE, PAR, RMINP, XZTHE, NS, NA, NPSI, INCEL,
1 NPCT, NPRET, DELTE, ST, SS, XC, IPSI, IPOTR, IPSVEC, PARW, IPRET,
2 ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
3 XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
4 ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
5 EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
6 DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
  PSINC(1,1)=1.0
  PSINC(1,2)=0.0
  PSINC(1,3)=0.0
  PSINC(2,1)=0.0
  PSINC(2,2)=COSF(APSI)
  PSINC(2,3)=SINF(APSI)
  PSINC(3,1)=0.0
  PSINC(3,2)=-PSINC(2,3)
  PSINC(3,3)=PSINC(2,2)
  I=IPSVEC(1,JJ)
  DO 2 K=1, 3
2 XZPSI(K,JJ)=XC(K,I)
  K=IPSVEC(2,JJ)
  CALL VS(XC(1,K),XC(1,I),V1)
  CALL NORM(V1,A1(1,1))
  IF (ABSF(V1(2))+ABSF(V1(3))) 3, 3, 4
3 CALL VXV(V1,YV,V2)
  GO TO 5
4 CALL VXV(V1,XV,V2)
5 CALL NCRM(V2,A1(1,2))
  CALL VXV(A1(1,1),A1(1,2),A1(1,3))
  CALL GINV3(A1,A2,NG)
  CALL MM(PSINC,A2,A3)
  CALL MM(A1,A3,RTPSI(1,1,JJ))
9 RETURN
  END
END ACCNTA0015 @D.WILLIAMS@ PCCG
START ACCNTA0015 @D.WILLIAMS@ PCCG

```

```

CCMPLE  RUN  FORTRAN LIST
C  SUBROUTINE DJKL1  ROTATION PARAMETER
  SUBROUTINE DJKL1(ITABW,JKTAB,XC,PARW,SS,STWE,XZTHE,ITHE,IPRET,
1  IPCTR, E)
  DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
1  STWE(3,200),XZTHE(3,2), ITHE(100), IPRET(8,8), IPCTR(100)
  DIMENSION R(3,3,2), V1(3), V2(3), V3(3)
  E=C.0
  R(1,2,1)=-PARW(3)
  R(1,3,1)= PARW(2)
  R(2,3,1)=-PARW(1)
  R(1,2,2)=-PARW(9)
  R(1,3,2)= PARW(8)
  R(2,3,2)=-PARW(7)
  DO 2  J=1, 2
  DO 2  K=1, 3
  DO 1  KK=K, 3
1  R(KK,K,J)=-R(K,KK,J)
2  R(K,K,J)=1.0
  DO 3  I=1, ITABW
  IA=JKTAB(1,I)
  IB=JKTAB(2,I)
  LTS=JKTAB(3,I)
  LSS=JKTAB(4,I)
  IARB=ITHE(IA)
  IBRB=ITHE(IB)
  CALL VS(XC(1,IA),XZTHE(1,IARB),V1)
  CALL MV(R(1,1,IARB),V1,V2)
  CALL VA(V2,XZTHE(1,IARB),V1)
  CALL VS(XC(1,IB),XZTHE(1,IBRB),V2)
  CALL MV(R(1,1,IBRB),V2,V3)
  CALL VA(V3,XZTHE(1,IBRB),V2)
  CALL MV(SS(1,1,LSS),V2,V3)
  CALL VA(STWE(1,LTS),V3,V2)
  CALL MAG(V1,V2,DIST)
  CALL EJKL(I,DIST,PARW,JKTAB,IPRET,IPCTR,C1)
  E=E+C1
3  CONTINUE
  RETURN
  END

END      ACCNTA0015  @D.WILLIAMS2
START    ACCNTA0015  @D.WILLIAMS2
CCMPLE  RUN  FORTRAN LIST
C  SUBROUTINE DJKL2  TRANSLATION PARAMETER
  SUBROUTINE DJKL2(ITABW,JKTAB,XC,PARW,SS,STWE,ITHE,IPRET,IPCTR,E)
  DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
1  STWE(3,200),ITHE(100), IPRET(8,8), IPCTR(100)
  DIMENSION V1(3),V2(3),V3(3)
  E=C.0
  DO 1  I=1, ITABW
  IA=JKTAB(1,I)
  IB=JKTAB(2,I)
  LTS=JKTAB(3,I)
  LSS=JKTAB(4,I)
  IARB=ITHE(IA)*6-2
  IBRB=ITHE(IB)*6-2
  CALL VA(XC(1,IA),PARW(IARB),V1)
  CALL VA(XC(1,IB),PARW(IBRB),V2)
  CALL MV(SS(1,1,LSS),V2,V3)
  CALL VA(STWE(1,LTS),V3,V2)

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CALL MAG(V1,V2,DIST)
CALL EJKL(I,DIST,PARW,JKTAB,IPRET,IPOTR,C1)
E=E+C1
1 CONTINUE
RETURN
END

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```

END      ACCNTAOC15 @D.WILLIAMS@
START   ACCNTAOC15 @D.WILLIAMS@
CCMPIL  RUN  FORTRAN LIST
C       SUBRCUTINE DJKL3  SUBROTATION PARAMETER
        SUBRCUTINE DJKL3(ITABW,JKTAB,XC,PARW,SS,STWE,IPSI,RTPSI,XZPSI,
1  IPRET,IPCTR,J,E)
        DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
1  STWE(3,200), IPSI(100), RTPSI(3,3,12), XZPSI(3,12), IPRET(8,8),
1  IPCTR(100)
        DIMENSION V1(3), V2(3), V3(3)
        E=0.0
        JPSI=J-12
        DO 10 I=1, ITABW
          IA=JKTAB(1,I)
          IB=JKTAB(2,I)
          LTS=JKTAB(3,I)
          LSS=JKTAB(4,I)
          IAP=IPSI(IA)
          IBP=IPSI(IB)
          IF (IAP-JPSI) 1, 2, 1
1        DO 3 N=1, 3
3          V1(N)=XC(N,IA)
          GO TO 4
2        CALL VS(XC(1,IA),XZPSI(1,IAP),V1)
          CALL MV(RTPSI(1,1,IAP),V1,V2)
          CALL VA(V2,XZPSI(1,IAP),V1)
4        IF (IBP-JPSI) 5, 6, 5
5        DO 7 N=1, 3
7          V2(N)=XC(N,IB)
          GO TO 8
6        CALL VS(XC(1,IB),XZPSI(1,IBP),V2)
          CALL MV(RTPSI(1,1,IBP),V2,V3)
          CALL VA(V3,XZPSI(1,IBP),V2)
8        CALL MV(SS(1,1,LSS),V2,V3)
          CALL VA(STWE(1,LTS),V3,V2)
          CALL MAG(V1,V2,DIST)
          CALL EJKL(I,DIST,PARW,JKTAB,IPRET,IPOTR,C1)
          E=E+C1
10       CONTINUE
RETURN
END

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END      ACCNTACC15 @D.WILLIAMS@
START   ACCNTAOC15 @D.WILLIAMS@
CCMPIL  RUN  FORTRAN LIST
C       SUBRCUTINE DJKL4  LATTICE PARAMETER
        SUBRCUTINE DJKL4(ITABW,JKTAB,XC,PARW,SS,STWE,DINV,IPRET,IPCTR,E)
        DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
1  STWE(3,200), DINV(3,3), IPRET(8,8), IPCTR(100)
        DIMENSION A1(3,3), V1(3), V2(3), V3(3), DINC(3,3)
        E=C.C
        CALL ORMAT(PARW(25),DINC)
        CALL MM(DINC,DINV,A1)

```

```

DO 1 I=1, ITARh
IA=JKTAB(1,I)
IB=JKTAB(2,I)
LTS=JKTAB(3,I)
LSS=JKTAB(4,I)
CALL MV(A1,XC(1,IA),V1)
CALL MV(XC(1,IB),V2)
CALL MV(LSS(1,1,LSS),V2,V3)
CALL VA(STWE(1,LTS),V3,V2)
CALL MAG(V1,V2,DIST)
CALL EJKL(I,DIST,PARh,JKTAB,IPRET,IPOTR,C1)
E=E+C1
1 CONTINUE
RETURN
END

```

Page 29, lines 7, 8 and 9 should be:

```

CALL MV(SS(1,1,LSS),XC(1,IB),V2)
CALL VA(STWE(1,LTS),V2,V3)
CALL MV(A1,V3,V2)

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END      ACCNTA0015  @D.WILLIAMS@
START    ACCNTA0015  @D.WILLIAMS@
CCMPILE  RLN  FORTRAN LIST
C        SUBROUTINE RCTCR(A,B)  OBTAIN ORTHONORMALIZED ROTATION MATRIX
SUBROUTINE RCTCR(A,B)
DIMENSION A(3), B(3,3)
THETA=SQRTF(1.C-0.25*(A(1)*A(1)+A(2)*A(2)+A(3)*A(3)))
XI=0.5*A(1)
ETA=0.5*A(2)
ZETA=0.5*A(3)
B(1,1)=XI*XI-ETA*ETA-ZETA*ZETA+THETA*THETA
B(2,1)=2.0*(XI*ETA+ZETA*THETA)
B(3,1)=2.0*(XI*ZETA-ETA*THETA)
B(1,2)=2.0*(XI*ETA-ZETA*THETA)
B(2,2)=-XI*XI+ETA*ETA-ZETA*ZETA+THETA*THETA
B(3,2)=2.0*(ETA*ZETA+XI*THETA)
B(1,3)=2.0*(XI*ZETA+ETA*THETA)
B(2,3)=2.0*(ETA*ZETA-XI*THETA)
B(3,3)=-XI*XI-ETA*ETA+ZETA*ZETA+THETA*THETA
RETURN
END

END      ACCNTA0015  @D.WILLIAMS@
START    ACCNTA0015  @D.WILLIAMS@
COMPILE  RUN  FORTRAN LIST
C        INVERT 3X3 MATRIX
SUBROUTINE GINV3(A,B,NG)
DIMENSION A(3,3), B(3,3)
C=A(1,1)*A(2,2)*A(3,3)-A(2,3)*A(3,2)
1 -A(1,2)*A(2,1)*A(3,3)-A(2,3)*A(3,1)
2 +A(1,3)*A(2,1)*A(3,2)-A(2,2)*A(3,1)
IF (ABSF(D)-10.0E-25) 2, 2, 1
2 NG=1
GO TO 99
1 C=1.C/C
B(1,1)=C*(A(2,2)*A(3,3)-A(2,3)*A(3,2))
B(2,1)=C*(A(2,3)*A(3,1)-A(2,1)*A(3,3))
B(3,1)=C*(A(2,1)*A(3,2)-A(2,2)*A(3,1))
B(1,2)=C*(A(1,3)*A(3,2)-A(1,2)*A(3,3))
B(2,2)=C*(A(1,1)*A(3,3)-A(1,3)*A(3,1))
B(3,2)=C*(A(1,2)*A(3,1)-A(1,1)*A(3,2))
B(1,3)=C*(A(1,2)*A(2,3)-A(1,3)*A(2,2))
B(2,3)=C*(A(1,3)*A(2,1)-A(1,1)*A(2,3))
B(3,3)=C*(A(1,1)*A(2,2)-A(1,2)*A(2,1))

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NG=C
99  RETLRN
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END      ACCNTA0015 @D.WILLIAMS@
START    ACCNTA0015 @D.WILLIAMS@
CCMPILE  RLN  FORTRAN LIST

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C  SUBRCUTINE ORMAT
   SUBRCUTINE ORMAT(ALAT,DMAT)
   DIMENSION ALAT(6), DMAT(3,3)
   SIN6=SINF(ALAT(6))
   COS5=CCSF(ALAT(5))
   COS4=COSF(ALAT(4))
   COS6=CCSF(ALAT(6))
   VV=1.0-COS4*COS4-CCS5*COS5-COS6*COS6+2.C*COS4*COS5*COS6
   VV=SQRTF(VV)
   CMAT(1,1)=ALAT(1)*SIN6
   CMAT(1,2)=C.0
   V=(COS5-CCS4*CCS6)/SIN6
   CMAT(1,3)=ALAT(3)*V
   CMAT(2,1)=ALAT(1)*COS6
   CMAT(2,2)=ALAT(2)
   CMAT(2,3)=ALAT(3)*COS4
   CMAT(3,1)=C.0
   DMAT(3,2)=0.0
   CMAT(3,3)=ALAT(3)*VV/SIN6
   RETURN
   END

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```

END      ACCNTA0015 @D.WILLIAMS@
START    ACCNTA0015 @D.WILLIAMS@
CCMPILE  RLN  FORTRAN LIST

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C  SUBROUTINE MM(A,B,C)
   SUBROUTINE MM(A,B,C)
   DIMENSION A(3,3), B(3,3), C(3,3)
   DO 1 I=1, 3
   DO 1 J=1, 3
   C(I,J)=0.0
   DO 1 K=1, 3
1  C(I,J)=C(I,J)+A(I,K)*B(K,J)
   RETURN
   END

```

```

START    ACCNTA0015 @D.WILLIAMS@
CCMPILE  RLN  FORTRAN LIST

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C  SUBROUTINE MV(A,B,C)
   SUBROUTINE MV(A,B,C)
   DIMENSION A(3,3), B(3), C(3)
   DO 1 I=1, 3
   C(I)=0.0
   DO 1 J=1, 3
1  C(I)=C(I)+A(I,J)*B(J)
   RETURN
   END

```

```

END      ACCNTA0015 @D.WILLIAMS@
START    ACCNTA0015 @D.WILLIAMS@
CCMPILE  RLN  FORTRAN LIST

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C   SUBRCUTINE VA(A,B,C)
      SUBRCUTINE VA(A,P,C)
      DIMENSION A(3), B(3), C(3)
      DO 1 I=1, 3
1  C(I)=A(I)+B(I)
      RETURN
      END

      END          ACCNTAOC15 @D.WILLIAMS@
      START       ACCNTAOC15 @D.WILLIAMS@
      CCMPLE      RUN FORTRAN LIST
C   SUBROUTINE VS(A,B,C)
      SUBRCUTINE VS(A,B,C)
      DIMENSION A(3), B(3), C(3)
      DO 1 I=1, 3
1  C(I)=A(I)-B(I)
      RETURN
      END

      END          ACCNTAOC15 @D.WILLIAMS@
      START       ACCNTAOC15 @D.WILLIAMS@
      CCMPLE      RUN FORTRAN LIST
C   SUBROUTINE VXV(A, B, C)
      DIMENSION A(3), B(3), C(3)
      C(1)=A(2)*B(3)-A(3)*B(2)
      C(2)=A(3)*B(1)-A(1)*B(3)
      C(3)=A(1)*B(2)-A(2)*B(1)
      RETURN
      END

      END          ACCNTAOC15 @D.WILLIAMS@
      START       ACCNTAOC15 @D.WILLIAMS@
      CCMPLE      RUN FORTRAN LIST
C   SUBROUTINE NORM(A,B)
      SUBRCUTINE NORM(A,B)
      DIMENSION A(3), B(3)
      C1=SQRTF(A(1)*A(1)+A(2)*A(2)+A(3)*A(3))
      DO 1 I=1, 3
1  B(I)=A(I)/C1
      RETURN
      END

      END          ACCNTAOC15 @D.WILLIAMS@
      START       ACCNTAOC15 @D.WILLIAMS@
      CCMPLE      RUN FORTRAN LIST
C   SUBROUTINE MAG(A,B,DIST)
      SUBRCUTINE MAG(A,B,DIST)
      DIMENSION A(3), B(3)
      DO 1 I=1, 3
1  A(I)=A(I)-B(I)
      DIST=SQRTF(A(1)*A(1)+A(2)*A(2)+A(3)*A(3))
      RETURN
      END

      END          ACCNTAOC15 @D.WILLIAMS@
      START       ACCNTAOC15 @D.WILLIAMS@
      CCMPLE      RUN FORTRAN LIST

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C      SUBROUTINE FJKL(I,LIST,PARW,JKTAB,IPRET,IPCTR,C1)
C      SUBROUTINE FJKL(I,CIST,PARW,JKTAB,IPRET,IPCTR,C1)
C      DIMENSION PARW(90), JKTAB(4,1800), IPRET(8,8), IPCTR(100)
C      IA=JKTAB(1,I)
C      IB=JKTAB(2,I)
C      J=IPCTR(IA)
C      K=IPCTR(IB)
C      IP=IPRET(J,K)
C      N=27+4*IP
C      C1=PARW(N+3)*PARW(N+2)/PARW(N+1)
C      C2=(PARW(N+1)-CIST)/PARW(N+2)
C      C2=C1*EXP(C2)
C      C3=(PARW(N+1)/CIST)**PARW(N+3)
C      C1=PARW(N)*(C3-C2)/(1.0-C1)
C      RETURN
C      END

END          ACCNTAOC15 @C.WILLIAMS@
START       ACCNTAOC15 @C.WILLIAMS@
CCMPLE     RUN  FORTRAN LIST
C          SUBROUTINE OUTPT
C          INPUT IS CNE CCNTRCL CARD FORMAT(2F10.2,10I5,I2)
C          COL. 1-10  CLIST - LIST DISTANCES THIS MUCH OR LESS THAN DOJK
C          COL. 11-20 BTEMP - TEMPERATURE FACTOR FOR LSSF CARDS
C          COL. 71-72 ICARD -  =0 FOR NO CARDS OUTPUT
C                               =1 FOR RECYCLE CARDS
C                               =2 FOR BOTH RECYCLE CARDS AND LSSF CARDS
C
C          SUBROUTINE OUTPT
C          DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
C          1  SS(3,3,24), XC(3,100), IPSI(100), IPCTR(100), IPSVEC(2,12),
C          2  PARW(90), IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
C          3  V2(3), V3(3), V4(3), V5(3), A1(3,3), A2(3,3), A3(3,3), XTRAN(3,2),
C          4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200), ISEL(90),
C          5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
C          6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
C          COMMON NINP, NCUT, TITLE, PAR, RMINP, XZTHE, NS, NA, NPSI, INCEL,
C          1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPCTR, IPSVEC, PARW, IPRET,
C          2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
C          3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
C          4  ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, CIST,
C          5  EZERC, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
C          6  DER, PINC, GRAD2, SHIFT, KSTCP, NG, NTHE, E, RMINC, NPMAX
C          DIMENSION NF(8), JF(8)
C          OUTPUT STWE TABLE FOR REFERENCE
C          71 FORMAT(1H0 40H  TRANSLATIONS LISTED IN STWE TABLE      /1H0
C          1      40H          LTS          X          Y          Z      /1H
C          2  /((1H I10,3F10.2))
C          WRITE OUTPUT TAPE NGUT, 71, ((STWE(I,J),I=1,3),J=1,LTSM)
C          1 FORMAT(1H0 12H  DISTANCES F5.2,25H OR MORE LESS THAN DOJK /1H0
C          1  50H  IA  IB  LTS  LSS  DOJK      ECJK      DELTA /1H )
C          2 FORMAT(1H 415,3F10.2)
C          3 FORMAT(F10.2,F10.2,10I5,I2)
C          READ INPUT TAPE NINP, 3, DLIST, BTEMP, (NF(I), JF(I), I=1, 5),
C          1  ICARD
C          WRITE OUTPUT TAPE NGUT, 1, DLIST
C          CO 4  I=1, ITABW
C          IA=JKTAB(1,I)
C          IB=JKTAB(2,I)
C          LTS=JKTAB(3,I)
C          LSS=JKTAB(4,I)

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J=IPCTR(IA)
K=IPCTR(IB)
IP=IPRFT(J,K)
DOJK=PAR(4*IP+28)
DCJK=DCSTE(2,I)
IF (DOJK-DCJK-CLIST) 4,6,6
6 DELTA=CCJK-DOJK
WRITE OUTPLT TAPE NOUT, 2, IA, IB, LTS, LSS, DOJK, DCJK, DELTA
4 CONTINUE
11 FORMAT(1HC 25H INITIAL ROTATION MATRIX/1H (/1H 3F10.5))
12 FORMAT(1HO 11H XZTHE(1)=F6.2, 11H XZTHE(2)=F6.2, 11H XZTHE(3)=
1 F6.2)
DO 53 K=1, NTHE
WRITE OUTPLT TAPE NOUT, 11, ((RMINP(I,J,K),J=1,3),I=1,3)
53 WRITE OUTPLT TAPE NOUT, 12, (XZTHE(I,K),I=1,3)
13 FORMAT(1HC 20H LATTICE CONSTANTS 3F10.4,3F10.2)
DO 14 I=28, 30
14 PAR(I)=PAR(I)+57.29578
WRITE OUTPLT TAPE NOUT, 13, (PAR(I),I=25,30)
18 FORMAT(1HC 25H POTENTIAL PARAMETERS /1H (/1H 4F10.5))
WRITE OUTPLT TAPE NOUT, 18, (PAR(I),I=31, NPMAX)
IF (ICARD) 61, 61, 62
32 FORMAT(14A5,A2)
62 PUNCH 32, (TITLE(I),I=1,15)
31 FORMAT(3F10.4,3F10.2)
PUNCH 31, (PAR(I),I=25,30)
34 FORMAT(4F10.5)
PUNCH 34, (PAR(I),I=31,NPMAX)
33 FORMAT(3F10.3,4I10)
PUNCH 33, ((XC(J,I),J=1,3),ITHE(I),IPSI(I),IPCTR(I),I=1,NA)
61 CONTINUE
C LIST OF COORDINATES FOR THE ATOMS, HYBL LSSF FORMAT
21 FORMAT(1HO 50H ATOM CARTESIAN CELL
1 /1H 50H IA X Y Z X
2 /1H 15H Y Z /1H )
22 FORMAT(1H 15,3F10.2,3F10.5)
WRITE OUTPLT TAPE NOUT, 21
DO 23 IA=1, NA
CALL MV(DINV,XC(1,IA),V1)
WRITE OUTPLT TAPE NOUT, 22, IA, (XC(I,IA),I=1,3), (V1(I),I=1,3)
24 FORMAT(2H103F10.5,F10.5,7X,3H1.0 7X,4H1.013X,1X,15)
IF (ICARD-2) 23, 63, 23
63 PUNCH 24, (V1(I),I=1,3), BTEMP, IA
23 CONTINUE
RETURN
END

END ACCNTAOC15 @D.WILLIAMS@ PCGC
START ACCNTAOC15 @D.WILLIAMS@ PCGC
CCMPILE RLN FORTRAN LIST PCGC
C SUBRCUTINE PATCH(PARW) SET DEPENDENT PARAMETERS
SUBRCUTINE PATCH(PARW)
DIMENSION PARW(9C)
RETURN
END

END ACCNTAOC15 @D.WILLIAMS@ PCGC

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