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LOS ALAMOS SCIENTIFIC LABORATORY
LOS ALAMOS ██████████ of the ██████████ NEW MEXICO
University of California

An Integrated Series of Crystallographic
Computer Programs
VII. Interatomic Distance and Angle Calculations

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An Integrated Series of Crystallographic
Computer Programs
VII. Interatomic Distance and Angle Calculations

by

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Abstract

The procedures employed and the computer program used for determining the distances between atoms in a unit cell are described. Any three atoms may be characterized by two vectors, each with an end common to one of the three atoms. The program may also be used to determine the angle between these two vectors.

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Introduction to the Series of Reports

The program described in this report is one of an integrated series of crystallographic computer programs. This series encompasses the entire subject of single-crystal structure analysis and includes programs for such items as:

- (1) crystal orientation for the collection of intensity data
- (2) processing of collected data to allow correction for Lorentz-polarization, absorption, background, and crystal-shape effects
- (3) comparison of processed data over equivalent reflections to ascertain the general validity of the data and to obtain a set of relative F^2 (F has the conventional structure factor meaning)
- (4) a Fourier series analysis coupled with a plotting routine for obtaining Patterson vector maps and electron density maps of the Fourier and difference Fourier types
- (5) a least-squares procedure for determining the positions and thermal motions (isotropic and/or anisotropic) of the atoms in a single crystal
- (6) various subroutines (two per space group) for the least-squares procedure

(7) miscellaneous procedures employed during and after a structure analysis, e. g., calculation of interatomic distances and angles, of the orientation relationship of thermal ellipsoid axes to the crystallographic axes of the crystal, of the polyhedral coordination of atoms; and the ordering of calculated and observed structure factors to prepare tables for publication.

Since each of the above items involves many repetitious procedures and calculations, it has been the authors' philosophy to employ computer techniques wherever possible and as early in the process of a structure determination as it is feasible to do so. Following this philosophy greatly reduces manual labor, minimizes clerical errors, and allows the maximum information to be obtained from the data.

Introduction to the Present Report

After the structure of a crystal has been determined, it is normally desirable to calculate the interatomic distances, provided this has not been done as part of the structure determination. These calculated distances may then be compared with known interatomic distances in other, similar, crystal structures as a check on the validity of the newly determined structure. Not infrequently a structure may refine in a proper manner but then must be rejected owing to a number of excessively short bonds. As a corollary to the calculation of chemical bond distances, the determination of the angles formed between various atoms may be very useful in assessing the correctness of a crystal structure. This report

lists the FØRTRAN II and FAP programs and describes their use in determining interatomic distances and angles.

The operating deck consists of a general program, DISAGL, and six subroutines: CØNTRL, CELØØØ, SYMØPR, ØPERTR, ASIN, and UNLØAD. These programs are listed and described in a later section of this report.

DISAGL reads control data from cards in the Monitor deck and experimental data either from cards in the Monitor deck or from a separate magnetic tape. On cards, the experimental data consist of unit cell parameters, unit cell contents, standard deviations of cell constants and atom positions, and problem identification. On magnetic tape, the experimental data consist of this same information plus the parameter correlation matrix, scale, and extinction parameters. The magnetic tape is usually prepared by our least-squares program (IA-3259) on logical tape unit 3(B3).

The program is normally run through the Monitor system. Following is a description of the complete Monitor deck.

* I. D. (Monitor Identification Card)

* XEQ (Monitor Card)

Binary cards for DISAGL

Binary cards for CØNTRL

Binary cards for CELØØØ

Binary cards for SYMØPR

Binary cards for ØPERTR

Binary cards for ASIN

Binary cards for UNLØAD

} from a compilation
of
FØRTRAN II
and
FAP
programs

* DATA (Monitor Card)

Control Cards

Experimental Data cards (if tape input is not used)

END. OF JOB (Monitor Card)

Mathematical Equations

The interatomic distance between two atoms located at x_1, y_1, z_1 and x_2, y_2, z_2 in any unit cell is given by

$$d = \left[(\Delta X \cdot a)^2 + (\Delta Y \cdot b)^2 + (\Delta Z \cdot c)^2 + 2(\Delta X \cdot \Delta Y \cdot a \cdot b \cdot \cos \lambda + \Delta X \cdot \Delta Z \cdot a \cdot c \cdot \cos \beta + \Delta Y \cdot \Delta Z \cdot b \cdot c \cdot \cos \alpha) \right]^{\frac{1}{2}}$$

where $\Delta X = x_2 - x_1$

$\Delta Y = y_2 - y_1$

$\Delta Z = z_2 - z_1$

and the other terms have their usual crystallographic meanings.

The standard deviation of the interatomic distance, σ_d , is given by

$$\sigma_d = \left(\sum_{i=1}^{12} \sum_{j=1}^{12} \frac{\partial d}{\partial \xi_i} \cdot \frac{\partial d}{\partial \xi_j} \cdot \sigma_i \cdot \sigma_j \cdot p_{ij} \right)^{\frac{1}{2}}$$

where $\frac{\partial d}{\partial \xi_i}$ is the partial derivative of the equation for interatomic distance, d , with respect to one of the twelve variables, ξ_i or j , which are

$x_1 y_1 z_1$

$x_2 y_2 z_2$

a b c

and

$\alpha, \beta, \gamma;$

σ_i or σ_j is the standard deviation of the individual parameter
i or j; and

ρ_{ij} is the correlation term between parameters i and j.

The vertex angle formed by two vectors is determined by the law of
cosines as follows:

$$\cos (213) = \frac{(d_{12})^2 + (d_{13})^2 - (d_{23})^2}{2(d_{12} \cdot d_{13})}$$

The standard deviation of the cosine of the angle 213 is given by
an equation having the same general form as that used for the standard
deviation of the interatomic distance. Only in the case of the angle,
the partial derivatives are obtained by differentiating the $\cos (213)$
equation, and the summation occurs over 15 variables instead of 12. The
extra three variables are the $x_3 y_3 z_3$ positions of atom 3. Prior to out-
put, the standard deviation of the angle 213 is obtained from the stand-
ard deviation of the cosine.

Glossary of Program Terms

For DISAGL:

COR (19306)

Storage field for correlation matrix read from
output of GENLES program

ICØ (15)	Storage field for control numbers for ØPERTR
ITHEX (192)	Control for calculation of derivatives of positional parameters in hexagonal system
IX (192)	Signed derivative count used for application of the correct algebraic sign to a correlation term for an X position
IY (192)	Signed derivative count used for application of the correct algebraic sign to a correlation term for a Y position
IZ (192)	Signed derivative count used for application of the correct algebraic sign to a correlation term for a Z position
J	General indexing variable
IL	Indexing variable used in operation of symmetry related positions
ØR	Origin choice for a space group
NSPG	Space group number
SD (196)	Storage field for standard deviations read from output of GENLES program
SX (192), SY (192), SZ (192)	Standard deviations of positional parameters x,y,z
X (192)	Positional parameters relative to <u>a</u> axis generated by symmetry operations
Y (192)	Positional parameters relative to <u>b</u> axis generated by symmetry operations
Z (192)	Positional parameters relative to <u>c</u> axis generated by symmetry operations
BIJ (6)	Storage for thermal parameters
CØ (225)	Storage field for covariance matrix
CØV (225)	Temporary storage field for covariance matrix
D2 (20)	Storage for vectors used in angle calculations

DAG2 (90)	Storage field for special angle DMAX
DER (36)	Derivative storage field
DER2 (240)	Storage field for derivatives of distances relative to x,y,z for use in angle calculations
IAT2 (20)	Storage for nonvertex atom count
IC (24)	Parameter count of x,y,z read from GENLES
IHEX2 (20)	Storage field for values of IHEX used in calculation of angles
ITY2 (20)	Index of the name of the nonvertex atom
IX1 (90), IY1 (90), IZ1 (90)	Least-squares parameter number counts read from the output tape from GENLES
NA (6)	Number of atoms of each type
PROBLM (12)	Problem identification
SIG (15)	Standard deviations of parameters that are utilized in calculation of an interatomic distance and angles
SIG2 (120)	Standard deviations of positional parameters x,y,z that are saved for angle calculations
SX1 (90), SY1 (90), SZ1 (90)	Standard deviations of X1, Y1, Z1
TYPE (12)	Storage field for atom names
X1 (90), Y1 (90), Z1 (90)	x,y,z positional parameters as read into the program
X2 (20), Y2 (20), Z2 (20)	x,y,z positional parameters that are saved for angle calculation
XID (15)	Parameter count from GENLES tape of positions used in both distance and angle calculations
XID2 (120)	Parameter count of quantities saved for angle calculations
A,B,C	Unit cell axes

ACELL, BCELL, CCELL	Floating point description of unit cell in which atom 2 lies
ANG	Angle between two vectors
CA, CB, CC	α , β , γ or $\cos \alpha$, $\cos \beta$, $\cos \gamma$
D	Calculated interatomic distance
D12	Distance between atom 1 and atom 2 used in calculation of angles. Atom 1 is the vertex atom.
D13	Distance between atom 1 and atom 3 used in calculation of angles. Atom 1 is the vertex atom.
D23	Distance between atom 2 and atom 3 used in calculation of angles
D23SQ	$(D23)^2$
D12R, D13R, D23R	Numbers used in calculation of the derivatives of an angle relative to the input parameters, x,y,z
DAGL	Maximum lengths of vectors between which angles will be calculated for all atoms
DMAX	Maximum calculated interatomic distance that will be listed
DX, DY, DZ	Partial derivative of calculated distance d with respect to ΔX , ΔY , and ΔZ , respectively
I, I1, I2, I3	General indexing variable
I3CONT	Control for input tape 3 (B3)
IA	Number of vectors, surrounding an atom, between which angles will be calculated
IA1, IA2	Numbers used to control listing of atomic names and counts
IAGL	Number of special angles
ICA, ICB, ICC	Indices controlling identification of adjacent unit cells relative to the reference unit cell

ICAL, ICB1, ICC1	Identification of the adjacent unit cells
ICD	Control character governing use of tape 3 (B3) input
IH	Index equal to the j'th value from the IHEX table
IPAGE	Page count
J2	General indexing variable
JX	Count of x,y,z positions read in when ICD = 2
K	General indexing variable
L	General indexing variable
LINE	Line count
M	General indexing variable
N12	Dead storage for isotropic/anisotropic control character from GENLES
N3	Number of position sets read in
NCR	Size of correlation matrix to be read in from GENLES
NJ	Number of kinds of atoms
SIN	Sine of the angle between the two vectors
STD	Standard deviation of angle/distance
XA, YB, ZC	Components of a vector relative to the unit cell edges
For CONTROL:	
ISG, IS	Indexing variables
K	Same as NCR in DISAGL
M	Same as ICD in DISAGL
NSPGRP	Same as NSPG in DISAGL

For SYMØP:

I	General indexing variable
K	Same as NØR in DISAGL
L	Same as Ll in DISAGL
Ll, L2, L3, L4, L5, L6	General bookkeeping indices and variables
M	Same as ICP in DISAGL
NSPGRP	Same as NSPG in DISAGL

For CELØØØ:

L	Same as Ll in DISAGL
M (18)	Dummy variable

Data Cards and/or Tape Description

Data cards for DISAGL consist of one control card and cards containing the experimental data. The number of these cards (as outlined below) depends on whether all, or part, or none of the experimental data is to be read in on magnetic tape, tape 3(B3), prepared by GENLES (LA-3259). The minimum number of cards is two (Cards 1 and 2), the maximum depends on the particular problem under consideration.

Card 1: Contains the control characters NSPG, NØR, DMAX, DAGL, I3CØNT, IAGL, and ICD in format 2I5, 2F10.5, 3I5.

NSPG = space group number

NØR = origin choice

DMAX = largest calculated distance to be printed in output

DAGL = maximum length of vectors for angle calculations (If DAGL is greater than DMAX, then DAGL is the limit in distances to be listed.)

I3CØNT = 0, unload tape 3(B3) at end of run;
 = 1, do not unload tape 3(B3) at end of run.
 IAGL = number of atoms for special angle calculations
 ICD = 0, for all cell data on tape 3(B3);
 = 1, unit cell and contents on tape 10(A2). Standard
 deviations of positional parameters, correlation
 matrix, scale, and extinction parameters on tape
 3(B3). Read cards 4 through 7;
 = 2, no data on tape 3(B3). Read cards 4 through 9.

Card 2: Contains the standard deviations of the unit cell constants in
 format 6F10.5.

Card 3 needed only if IAGL is greater than 0.

Card 3: Contains the parameter set count of the vertex atom and the
 special angle $d_{\max}$ DAG2, in format 5(I5,F10.5). Five special
 sets may be placed per card. (If the general angle, DAGL, is
 greater than the special angle, DAG2, then the general angle
 DAGL is the limit in distances to be listed.)

Cards 4 through 7 needed only if ICD equals 1 or 2.

Card 4: Contains the unit cell constants $a, b, c, \alpha, \beta, \gamma$ in format 6F10.5.

Card 5: Contains the number of types of atoms (the maximum is six),
 the number of position sets for each of six types, and the
 number of x, y, z parameter sets to be read. Format 8I5.

Card 6: Contains the names of the different types of atoms in format

12A6. Each name must be no more than 12 characters in length.

Card 7: Contains the atomic coordinates, x,y,z, and the parameter number (see LA-3259) associated with the coordinates for a given atom in format 3F10.5, 3I5.

Special Note: The parameter numbers are to be used only if ICD = 1. If ICD = 2, the program sets up its own running account of those numbers and a card 8 is read after each card 7.

Cards 8 and 9 needed only if ICD = 2.

Card 8: Contains the standard deviations of the positional parameters for a given atom in format 3F10.5.

Card 9: Contains 72 Hollerith characters for problem identification.

Output Description

The output from DISAGL consists of an off-line printout containing the following information. The problem identification is listed followed by the name of the first atom, the name of the second atom, the identification of the unit cell in which the second atom lies, the distance in Å between atom 1 and atom 2, the standard deviation of this distance, the positional parameters of atom 1, and the positional parameters of atom 2. This information is repeated for all atom 2's having distances less than DMAX from atom 1. Then is listed angular information in the arrangement: end atom 1, vertex atom, end atom 2, the angle at the vertex, its standard deviation, the xyz position of end atom 1, the xyz position of the vertex atom, and the xyz position of end atom 2. This is repeated

for all angles having as vertex atom the first atom of the interatomic distance listing.

This double listing, distance and angle, is then repeated for each atom of each type given until the total number of atoms has been processed.

Illustrative Example: Input

As an illustrative example of the use of this program we will consider the determination of the interatomic distances and angles appropriate to the distorted octahedron found in the crystal structure of $\text{UO}_2(\text{OH})_2$, uranyl dihydroxide.* $\text{UO}_2(\text{OH})_2$ is orthorhombic, space group Pbca , No. 61, with $a = 5.635 \pm 0.007$, $b = 6.285 \pm 0.008$, and $c = 9.919 \pm 0.008$ Å, and contains four formula units per unit cell. Positional parameters are:

	Atom	X	Y	Z
	U	0	0	0
Uranyl	O	0.1370 ± 0.0090	0.4672 ± 0.0189	0.3348 ± 0.0049
Hydroxide	O	0.1848 ± 0.0094	0.2791 ± 0.0087	0.0925 ± 0.0047

Let us calculate all interatomic distances out to a maximum of 3.5 Å. For the general angle calculations let 3.0 Å be the maximum length of the angle vectors. No special angles whose vectors exceed the

*Roof, R. B., Jr., Cromer, D. T., and Larson, A. C. (1964). Acta Cryst. 17, 701.

3.0 Å of the general angle vectors need to be calculated. It is assumed that a tape 3 is not available for this material. Therefore, all the information must be read in on cards.

The information given in the proceeding paragraphs is collected on punched cards as described in the Data Card section and is illustrated in Fig. 1. Note that a type-7 card is followed by a type-8 card, i.e., the card containing the standard deviations of the positions follows the card containing the positions.

Illustrative Example: Output

Figure 2 is a reproduction of the first page of the listing of the output from the program DISAGL for the illustrative example. For a slightly distorted octahedron containing an atom at its center, there are, in general, six atomic distances and fifteen angles to be determined. If the octahedron contains a center of symmetry, however, there are only three different interatomic distances and six different angles. In addition there are three angles equal to 180° . The individual distances and angles are readily available from the self-explanatory columns given in Fig. 2.

[illegible]

Figure 1. Input Data Cards for the Illustrative Example.

INTERATOMIC DISTANCES AND ANGLES FOR U101210H12

PAGE 1

ATOM 1	ATOM 2	CELL	DISTANCE	STD.	X1	Y1	Z1	X2	Y2	Z2
URANIUM 1	URANYL 0	1 -1-1 0	1.82305	0.05051	0.	0.	0.	0.86300	0.96720	0.16520
URANIUM 1	URANYL 0	1 0 0-1	1.82305	0.05051	0.	0.	0.	0.13700	0.03280	0.83480
URANIUM 1	HYDROXIDE 3	1 -1-1-1	2.23673	0.05307	0.	0.	0.	0.81520	0.72090	0.90750
URANIUM 1	HYDROXIDE 3	1 -1 0-1	2.43394	0.05272	0.	0.	0.	0.68480	0.22090	0.90750
URANIUM 1	HYDROXIDE 3	1 0-1 0	2.43394	0.05272	0.	0.	0.	0.31520	0.77910	0.09250
URANIUM 1	HYDROXIDE 3	1 0 0 0	2.23673	0.05307	0.	0.	0.	0.18480	0.27910	0.09250

END ATOM 1	VERTEX ATOM	END ATOM 2	ANGLE	STD.	XYZ END ATOM 1	XYZ VERTEX ATOM	XYZ END ATOM 2
URANYL 0	1	URANIUM 1	130.00	-0.	-0.137-0.033 0.165	0.	0.137 0.033-0.165
URANYL 0	1	URANIUM 1	94.75	3.36	-0.137-0.033 0.165	0.	-0.185-0.279-0.093
URANYL 0	1	URANIUM 1	95.41	2.72	-0.137-0.033 0.165	0.	-0.315 0.221-0.093
URANYL 0	1	URANIUM 1	84.59	2.72	-0.137-0.033 0.165	0.	0.315-0.221 0.092
URANYL 0	1	URANIUM 1	85.25	3.36	-0.137-0.033 0.165	0.	0.185 0.279 0.092
URANYL 0	1	URANIUM 1	85.25	3.36	0.137 0.033-0.165	0.	-0.185-0.279-0.093
URANYL 0	1	URANIUM 1	84.59	2.72	0.137 0.033-0.165	0.	-0.315 0.221-0.093
URANYL 0	1	URANIUM 1	95.41	2.72	0.137 0.033-0.165	0.	0.315-0.221 0.092
URANYL 0	1	URANIUM 1	94.75	3.36	0.137 0.033-0.165	0.	0.185 0.279 0.092
HYDROXIDE 0	1	URANIUM 1	87.30	0.98	-0.185-0.279-0.093	0.	-0.315 0.221-0.093
HYDROXIDE 0	1	URANIUM 1	92.70	0.98	-0.185-0.279-0.093	0.	0.315-0.221 0.092
HYDROXIDE 0	1	URANIUM 1	179.99	0.00	-0.185-0.279-0.093	0.	0.185 0.279 0.092
HYDROXIDE 0	1	URANIUM 1	180.00	-0.	-0.315 0.221-0.093	0.	0.315-0.221 0.092
HYDROXIDE 0	1	URANIUM 1	92.70	0.98	-0.315 0.221-0.093	0.	0.185 0.279 0.092
HYDROXIDE 0	1	URANIUM 1	87.30	0.98	0.315-0.221 0.092	0.	0.185 0.279 0.092

Figure 2. Illustrative Example of Output from DISAGL.

FØRTRAN II Listings of Programs

On the following pages are the FØRTRAN II and FAP listings of the main program and the subroutines described in this report.

DISAGL is written in FØRTRAN II

CØNTRL is written in FØRTRAN II

CELØØØ is written in FØRTRAN II

SYMØPR is written in FØRTRAN II

ØPERTR is written in FAP

DISAGL is the main program and is responsible for calculation of inter-atomic distances and angles. CØNTRL calculates control numbers for the symmetry-generating subroutine SYMØPR. ØPERTR is used by SYMØPR to apply the symmetry elements calculated by CØNTRL to the given atomic positions. CELØØØ determines whether the atomic position under consideration lies in the initial unit cell or in unit cells adjacent to the initial unit cell. ASIN and UNLØAD are necessary minor subroutines that are listed and described in the fifth report of this series (IA-3259).

CDISAGL DISTANCE AND ANGLE PROGRAM
CCORDIS DISTANCE WITH CORRELATION TERMS

C DATA

C TAPE 3(B3) PREPARED BY LES.

C 2 CARDS

C CARD 1

C COLS 1-5 SPACE GROUP NO. FROM INT. TABLES(1952). I5
C COLS 6-10 ORIGIN CHOICE. I5
C COLS 11-20 DMAX, GREATEST DISTANCE TO BE PRINTED. F10.5
C COLS 21-30 DAGL, MAX. LENGTH OF VECTORS FOR ANGLE CALCNS. F10.5
C IF DAGL IS GREATER THAN DMAX, DAGL IS LIMIT.
C COLS. 31-35 I3CONT. I5
C I3CONT = 0 TO UNLOAD (3) AT END OF RUN
C I3CONT = 1 TO LEAVE LOGICAL TAPE 3 ON MACHINE
C COLS 36-40 NO. OF SPECIAL ANGLE DMAXS.
C COLS 41-45 0 FOR ALL CELL DATA ON TAPE 3.
C 1 CELL AND CONTENTS ON TAPE 10, SIGMAS, CORRELATION
C MATRIX, SCALE, AND EXTINCTION PARAMETERS ON 3,
C READ CARDS 4 THROUGH 7
C 2 NO DATA ON TAPE 3
C READ CARDS 4 THRU 9

C CARD 2. STANDARD DEV. OF CELL CONSTS. 6F10.5

C CARD 3 SPECIAL ANGLE LOCATIONS AND THEIR DMAXS.
C 5 SETS PER CARD AS 5(I5,F10.5)

C CARD 4 CELL CONSTANTS. 6F10.5

C CARD 5 NO. OF TYPES OF ATOMS, NO. OF EACH TYPE, NO. OF POSITION
C SETS. 8I5

C CARD 6 ATOMIC NAMES(I2A6)

C CARD 7 ATOMIC COORDINATES AND PARAMETER COUNT.(3F10.5,3I5)

C CARD 8 SIGMAX,SIGMAY,SIGMAZ(F10.5)

C CARD 9 PROBLEM IDENTIFICATION

COMMON NSPG,NOR,ICO,J,L1,X,Y,Z,IX,IY,IZ,IHXS,SX,SY,SZ,SD,COR
DIMENSION ICO(15),X(192),Y(192),Z(192),IX(192),IY(192),IZ(192),
1 COR(17306),X1(90),Y1(90),Z1(90),IX1(90),IY1(90),IZ1(90),
2 PROBLM(12),NA(6),SD(196),TYPE(12),BIJ(6),SX(192),SY(192),SZ(192),
3 SX1(90),SY1(90),SZ1(90),IC(24),COV(15,15),DER(36),SIG(15),XID(15)
4 ,X2(20),Y2(20),Z2(20),XID2(6,20),IHXS2(20),DER2(12,20),IAT2(20),
5 IHXS(192),O2(20),ITY2(20),CO(15,15),SIG2(6,20),DAG2(90)

1 FORMAT (2I5,2F10.5,8I5)

2 FORMAT (6F10.5)

3 FORMAT (1H12A6,30X4HPAGE13/1H06X6HATOM 110X6HATOM 25X4HCELL4X

1 15HDISTANCE STD.9X2HX16X2HY16X2HZ18X2HX26X2HY26X2HZ2//)

4 FORMAT (1H 2(2A6,I2,2X),3I2,F11.5,F9.5,2X2(2X3F8.5))

5 FORMAT (5(I5,F10.5))

```

6 FORMAT (118H- END ATOM 1 VERTEX ATOM END ATOM 2 ANGLE
1 STD. XYZ END ATOM 1 XYZ VERTEX ATOM XYZ END ATOM 2
2 //)
7 FORMAT (1H112A6,30X4HPAGEI3/118H0 END ATOM 1 VERTEX ATOM E
1ND ATOM 2 ANGLE STD. XYZ END ATOM 1 XYZ VERTEX ATOM
2 XYZ END ATOM 2 //)
8 FORMAT (3(1X2A6,I2),F8.2,F7.2,3(2X3F6.3))
9 FORMAT (6F10.5/8I5/12A6)
10 FORMAT(3F10.5,3I5)
11 FORMAT ( 12A6)

99 CONTINUE
DO 990 I=1,17306
990 COR(I) = 0.0
DO 991 I = 1,186
J = (I*(I+1))/2
991 COR(J) = 1.0
JX = 1
READ INPUT TAPE 10,1,NSPG,NOR,DMAX,DAGL,I3CONT,IAGL,ICD
DO 98 I=1,90
98 DAG2(I) = 0.0
READ INPUT TAPE 10,2,(SIG(I),I=7,12)
IF ( IAGL ) 96,96,97
97 READ INPUT TAPE 10,5,(I,(DAG2(I)),J=1,IAGL)
96 CONTINUE
IF (NSPG) 100,100,101
100 IF ( I3CONT ) 102,102,103
101 IF ( NSPG-230 ) 104,104,100
102 CALL UNLOAD(3)
103 GO TO 99
104 CONTINUE
CALL CONTRL
IF ( ICD-2 ) 1040,1051,1051
1040 CONTINUE
REWIND 3
READ TAPE 3,PROBLM,NCOR
L = 1
DO 105 I=1,NCOR
J = L+I-1
READ TAPE 3,(COR(K),K=L,J)
105 L = L+I
READ TAPE 3,(SD(I),I=1,NCOR)
IF ( ICD ) 1050,1050,1051
1050 CONTINUE
READ TAPE 3,A,B,C,CA,CB,CC,NJ,(NA(I),I=1,NJ),TYPE,N3
DO 106 I=1,N3
106 READ TAPE 3,X1(I),Y1(I),Z1(I),BIJ,N12,IX1(I),IY1(I),IZ1(I)
GO TO 1053
1051 READ INPUT TAPE 10,9,A,B,C,CA,CB,CC,NJ,NA,N3,TYPE
DO 1052 I = 1,N3
READ INPUT TAPE 10,10,X1(I),Y1(I),Z1(I),IX1(I),IY1(I),IZ1(I)
IF ( ICD-2 ) 1052,1060,1060
1060 IX1(I) = JX
IY1(I) = JX+1
IZ1(I) = JX+2
READ INPUT TAPE 10,10,SD(JX),SD(JX+1),SD(JX+2)
JX = JX+3
1052 CONTINUE
IF ( ICD-2 ) 1062,1061,1061
1061 NCOR = JX-1

```

```

      READ INPUT TAPE 10,11,PROBLM
1062 CONTINUE
      IF ( CA-1.0 ) 1055,1055,1054
1054 CA = COSF(CA/57.2957795)
1055 IF ( CB-1.0 ) 1057,1057,1056
1056 CB = COSF(CB/57.2957795)
1057 IF ( CC-1.0 ) 1053,1053,1058
1058 CC = COSF(CC/57.2957795)
1053 CONTINUE
      DO 107 I=1,225
107  CO(I) = 0.0
      DO 108 I=1,15
      XID(I)=0.0
108  CO(I,I) = 1.0
      IF ( NSPG-75 ) 113,109,109
109  SIG(8) = SIG(7)
      CO(7,8) = 1.0
      IF ( NSPG-195 ) 95,112,112
      95 IF ( NSPG-143 ) 113,110,110
110 IF ( NOR-1 ) 113,111,113
111 CO(10,11) = 1.0
      CO(10,12) = 1.0
      CO(11,12) = 1.0
      SIG(11) = SIG(10)
      SIG(12) = SIG(10)
112 CO(7,9) = 1.0
      CO(8,9) = 1.0
      SIG(9) = SIG(7)
113 DO 114 I=1,15
      DO 114 J=I,15
114  CO(J,I) = CO(I,J)
      DO 115 I=1,N3
      X(I) = X1(I)
      Y(I) = Y1(I)
      Z(I) = Z1(I)
      L1 = 2
      CALL CEL000
      X1(I) = X(I)
      Y1(I) = Y(I)
      Z1(I) = Z(I)
      J = IX1(I)
      SX1(I) = SD(J)
      J = IY1(I)
      SY1(I) = SD(J)
      J = IZ1(I)
      SZ1(I) = SD(J)
115 CONTINUE
      IPAGE = 1
      LINE = 61
      L = 2
      IT1 = 1
      IA1 = 0
      DO 600 K=1,N3
      IA = 0
      IA1 = IA1+1
      IF ( IA1-NA(IT1) ) 131,131,130
130 IT1 = IT1+1
      IA1 = 1
131 CONTINUE
      IT2 = 1

```

```

      IA2 = 0
      DO 500 I=1,N3
      X(1)=X1(I)
      Y(1)=Y1(I)
      Z(1)=Z1(I)
      IX(1) = IX1(I)
      IY(1) = IY1(I)
      IZ(1) = IZ1(I)
      SX(1) = SX1(I)
      SY(1) = SY1(I)
      SZ(1) = SZ1(I)
      IHEX(1) = 0
      J = 1
      CALL SYMOPR
      J = J-1
      IA2 = IA2+1
      IF ( IA2-NA(IT2) ) 122,122,121
121  IT2 = IT2+1
      IA2 = 1
122  CONTINUE
      DO 400 ICA = 1,3
      ICA1 = ICA-2
      ACEL = ICA-2
      DO 400 ICB = 1,3
      ICB1 = ICB-2
      BCEL = ICB-2
      DO 400 ICC = 1,3
      ICC1 = ICC-2
      CCEL = ICC-2
      DO 400 J2 = 1,J
      XA=(X1(K)-(X(J2)+ACEL))*A
      YB=(Y1(K)-(Y(J2)+BCEL))*B
      ZC=(Z1(K)-(Z(J2)+CCEL))*C
      D = SQRTF(XA**2+YB**2+ZC**2+2.0*(XA*YB*CC
1    +XA*ZC*CB+YB*ZC*CA))
      IF ( D-0.0001 ) 400,400,199
199  IF ( D-MAX1F(DMAX,DAGL,DAG2(K)) ) 200,200,400
200  DX = (XA*A+YB*A*CC+ZC*A*CB)/D
      DY = (YB*B+XA*B*CC+ZC*B*CA)/D
      DZ = (ZC*C+XA*C*CB+YB*C*CA)/D
      DER( 7) = (XA*(XA+YB*CC+ZC*CB))/A/D
      DER( 8) = (YB*(YB+XA*CC+ZC*CA))/B/D
      DER( 9) = (ZC*(ZC+XA*CB+YB*CA))/C/D
      DER(10) = YB*ZC/D
      DER(11) = XA*ZC/D
      DER(12) = XA*YB/D
      XID(1) =IX1(K)
      XID(2) =IY1(K)
      XID(3) =IZ1(K)
      XID(4) =IX(J2)
      XID(5) =IY(J2)
      XID(6) =IZ(J2)
      DO 250 I1 = 1,6
250  IC(I1) = ABSF(XID(I1))
      DO 251 M=1,12
      DO 251 L=1,12
251  COV(L,M) = CO(L,M)
      L = 0
      DO 210 I1=1,NCOR
      DO 209 I2=1,6

```

```

      IF ( I1-IC(I2) ) 209,201,209
201 DO 208 I3=1,6
      IF ( I1-IC(I3) ) 208,202,202
202 IF ( IC(I3) ) 208,208,203
203 M = L+IC(I3)
      COV(I2,I3) = SIGNF(COR(M),XID(I2)*XID(I3)*COR(M))
      COV(I3,I2) = COV(I2,I3)
208 CONTINUE
209 CONTINUE
210 L = L+1
      DER(1) = DX
      DER(2) = DY
      DER(3) = DZ
      IH = IHEX(J2)+1
      GO TO (211,212,213), IH
211 DER(4) = -CX
      DER(5) = -CY
      GO TO 214
212 DER(4) = -CY
      DER(5) = DX+DY
      GO TO 214
213 DER(4) = DX+DY
      DER(5) = -DX
214 CONTINUE
      DER(6) = -CZ
      SIG(1) = SX1(K)
      SIG(2) = SY1(K)
      SIG(3) = SZ1(K)
      SIG(4) = SX(J2)
      SIG(5) = SY(J2)
      SIG(6) = SZ(J2)
      STD = 0.0
      DO 220 L=1,12
      DO 220 M=1,12
220 STD = STD+DER(L)*DER(M)*SIG(L)*SIG(M)*COV(L,M)
      STD = SQRTF(STD)
      IF ( LINE-58 ) 231,231,230
230 WRITE OUTPUT TAPE 9,3,PROBLM,IPAGE
      LINE = 3
      IPAGE = IPAGE+1
231 LINE = LINE+1
      WRITE OUTPUT TAPE 9,4,TYPE(2*IT1-1),TYPE(2*IT1),IA1,
1 TYPE(2*IT2-1),TYPE(2*IT2),IA2,ICA1,ICB1,ICC1,D,STD,X1(K),Y1(K),
2 Z1(K),X(J2),Y(J2),Z(J2)
      IF ( D-MAX1F(DAGL,DAG2(K)) ) 300,300,400
300 IF ( IA-20 ) 303,400,400
303 IA = IA+1
      X2(IA) = X(J2)+ACEL
      Y2(IA) = Y(J2)+BCEL
      Z2(IA) = Z(J2)+CCEL
      D2(IA) = D
      IHEX2(IA) = IHEX(J2)
      DO 301 L=1,12
301 DER2(L,IA) = DER(L)
      DO 302 L=1,6
      SIG2(L,IA) = SIG(L)
302 XID2(L,IA) = XID(L)
      ITY2(IA) = IT2
      IAT2(IA) = IA2
400 CONTINUE

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```

500 CONTINUE
    IF ( IA-1 ) 601,601,501
501 WRITE OUTPUT TAPE 9,6
    LINE = LINE+4
    DO 550 I=2,IA
    DO 550 J=1,IA
    D12 = D2(I-1)
    D13 = D2(J)
    XA = (X2(I-1)-X2(J))*A
    YB = (Y2(I-1)-Y2(J))*B
    ZC = (Z2(I-1)-Z2(J))*C
    D23SQ = XA**2+YB**2+ZC**2+2.0*(XA*YB*CC+XA*ZC*CB+YB*ZC*CA)
    D23 = SQRTF(D23SQ)
    DO 502 L=1,225
502 COV(L) = CG(L)
    DO 503 L=1,15
503 XID(L) = 0.0
    DO 504 L=1,6
506 SIG(L) = SIG2(L,I-1)
504 XID(L) = XID2(L,I-1)
    DO 505 L=1,3
507 SIG(L+12) = SIG2(L+3,J)
505 XID(L+12) = XID2(L+3,J)
    DO 508 L=1,15
508 IC(L) = ABSF(XID(L))
    L = 0
    DO 514 I1=1,NCOR
    DO 513 I2=1,15
    IF ( I1-IC(I2) ) 513,509,513
509 DO 512 I3=1,15
    IF ( I1-IC(I3) ) 512,510,510
510 IF ( IC(I3) ) 512,512,511
511 M=L+IC(I3)
    COV(I2,I3) = SIGNF(COR(M),XID(I2)*XID(I3)*COR(M))
    COV(I3,I2) = COV(I2,I3)
512 CONTINUE
513 CONTINUE
514 L = L+I1
    D13R = 1.0/D13-D13/(D12*D12)+D23SQ/(D12*D12)/D13
    D12R = 1.0/D12-D12/(D13*D13)+D23SQ/(D13*D13)/D12
    D23R = 2.0*D23/D12/D13
    DX = A*(XA+YB*CC+ZC*CB)/D23
    DY = B*(YB+XA*CC+ZC*CA)/D23
    DZ = C*(ZC+XA*CB+YB*CA)/D23
    IH = IHEX2(I-1)+1
    GO TO (515,516,517),IH
515 DER(25) = DX
    DER(26) = CY
    GO TO 518
516 DER(25) = CY
    DER(26) = -DX-DY
    GO TO 518
517 DER(25) = -DX-DY
    DER(26) = CX
518 IH = IHEX2(J)+1
    GO TO (519,520,521),IH
519 DER(28) = -DX
    DER(29) = -DY
    GO TO 522
520 DER(28) = -DY

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```

      DER(29) = CX+CY
      GO TO 522
521  DER(28) = DX+CY
      DER(29) = -DX
522  DER(27) = CZ
      DER(30) = -CZ
      DER(31) = (XA*(XA+YB*CC+ZC*CB))/A/D23
      DER(32) = (YB*(YB+XA*CC+ZC*CA))/B/D23
      DER(33) = (ZC*(ZC+XA*CB+YB*CA))/C/D23
      DER(34) = YB*ZC/D23
      DER(35) = XA*ZC/D23
      DER(36) = XA*YB/D23
      DO 523 L=1,3
      DER(L) = (DER2(L,I-1)*D13R+DER2(L,J)*D12R)/2.0
      DER(L+3) = (DER2(L+3,I-1)*D13R-DER(L+24)*D23R)/2.0
      DER(L+6) = (DER2(L+6,I-1)*D13R+DER2(L+6,J)*D12R-DER(L+30)*D23R)/2.0
      DER(L+9) = (DER2(L+9,I-1)*D13R+DER2(L+9,J)*D12R-DER(L+33)*D23R)/2.0
523  DER(L+12) = (DER2(L+3,J)*D12R-DER(L+27)*D23R)/2.0
      STD = 0.0
      DO 524 L=1,15
      DO 524 M=1,15
524  STD = STD+CER(L)*DER(M)*SIG(L)*SIG(M)*COV(L,M)
      STD = SQRTF(STD)
      LINE = LINE+1
      IF ( LINE-60 ) 526,526,525
525  WRITE OUTPUT TAPE 9,7,PROBLM,IPAGE
      LINE = 4
      IPAGE = IPAGE+1
526  L = IY2(I-1)
      M = IY2(J)
      SIN = (D12**2+D13**2-D23SQ)/(2.0*D12*D13)
      ANG = 90.0-ASINF(SIN)*57.2957795
      STD = STD/SQRTF(1.0-SIN**2) *57.2957795
550  WRITE OUTPUT TAPE 9,8,TYPE(2*L-1),TYPE(2*L),IAT2(I-1),TYPE(2*IT1-1
1 ),TYPE(2*IT1),IA1,TYPE(2*M-1),TYPE(2*M),IAT2(J),ANG,STD,X2(I-1),
2 Y2(I-1),Z2(I-1),X1(K),Y1(K),Z1(K),X2(J),Y2(J),Z2(J)
      LINE = 61
600  CONTINUE
      IF (ICD-2) 100,99,100
601  WRITE OUTPUT TAPE 9,4
      LINE = LINE+1
      GO TO 600
      END

```


NSPGNO CALCULATES CONTROL NUMBERS FOR SYMMETRY GENERATOR

```

SUBROUTINE CONTRL
COMMON NSPGRP,K,M
DIMENSION M(15)
DO 300 IS=1,15
300 M(IS)=0
    ISG=NSPGRP/50+1
    IS =NSPGRP-50*(ISG-1)+1
    GO TO (400,401,402,403,404),ISG
400 IS=IS-1
    GO TO (1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,
    1 23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,
    2 43,44,45,46,47,48,49),IS
401 GO TO (50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,
    1 67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,
    2 87,88,89,90,91,92,93,94,95,96,97,98,99),IS
402 GO TO (100,101,102,103,104,105,106,107,108,109,110,111,112,113,
    1 114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,
    2 130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,
    3 145,146,147,148,149),IS
403 GO TO (150,151,152,153,154,155,156,157,158,159,160,161,162,163,
    1 164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,
    2 180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,
    3 195,196,197,198,199),IS
404 GO TO (200,201,202,203,204,205,206,207,208,209,210,211,212,
    1 213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,
    2 228,229,230),IS
2 M(1)=290
1 RETURN
3 M(1)=258
GO TO 1
4 M(1)=322
GO TO 1
5 M(2)=68
GO TO 3
6 M(1)=32
GO TO 1
7 M(1)=544
GO TO 1
8 M(2)=68
GO TO 6
9 M(2)=68
GO TO 7
10 M(2)=32
GO TO 2
11 M(2)=322
GO TO 2
12 M(3)=68
GO TO 10
13 M(2)=544
GO TO 2
14 M(2)=608
GO TO 2
15 M(3)=68
GO TO 13
16 M(2)=34
GO TO 3
17 M(1)=288
M(2)=546

```

```

      GO TO 1
18  M(1)=34
      M(2)=356
      GO TO 1
19  M(1)=550
      M(2)=356
      GO TO 1
20  M(3)=68
      GO TO 17
21  M(3)=68
      GO TO 16
22  M(4)=516
      GO TO 21
23  M(3)=580
      GO TO 16
24  M(3)=580
      GO TO 19
25  M(2)=34
      GO TO 6
26  M(2)=2
      GO TO 7
27  M(2)=34
      GO TO 7
28  M(2)=34
      M(1)=6
      GO TO 1
29  M(1)=36
      M(2)=546
      GO TO 1
30  M(1)=578
      M(2)=34
      GO TO 1
31  M(1)=2
      M(2)=550
      GO TO 1
32  M(1)=34
      M(2)=70
      GO TO 1
33  M(1)=546
      M(2)=100
      GO TO 1
34  M(1)=34
      M(2)=582
      GO TO 1
35  M(3)=68
      GO TO 25
36  M(3)=68
      GO TO 26
37  M(3)=68
      GO TO 27
38  M(3)=576
      GO TO 25
39  M(1)=576
      M(2)=34
      M(3)=66
      GO TO 1
40  M(3)=576
      GO TO 28
41  M(3)=576
      GO TO 32

```

```

42 M(4)=576
   GØ TØ 35
43 M(1)=34
   M(2)=1162
   M(3)=576
   M(4)=68
   GØ TØ 1
44 M(3)=580
   GØ TØ 25
45 M(3)=580
   GØ TØ 32
46 M(3)=580
   GØ TØ 28
47 M(3)=290
   GØ TØ 25
48 IF ( K-1 ) 1000,1048,2048
1048 M(3)=288
   GØ TØ 34
2048 M(3)=578
   M(2)=102
   GØ TØ 2
49 M(3)=256
   GØ TØ 27
50 IF ( K-1 ) 1000,1050,2050
1050 M(3)=288
   GØ TØ 32
2050 M(3)=102
   M(2)=36
   GØ TØ 2
51 M(3)=32
   M(2)=38
   GØ TØ 2
52 M(2)=38
   M(3)=578
   GØ TØ 2
53 M(3)=290
   GØ TØ 31
54 M(3)=544
   M(2)=38
   GØ TØ 2
55 M(3)=290
   GØ TØ 32
56 M(3)=102
   M(2)=518
   GØ TØ 2
57 M(2)=768
   M(3)=66
   GØ TØ 2
58 M(3)=290
   GØ TØ 34
59 IF ( K-1 ) 1000,1059,2059
1059 M(3)=324
   GØ TØ 25
2059 M(3)=6
   M(2)=96
   GØ TØ 2
60 M(3)=70
   M(2)=544
   GØ TØ 2
61 M(3)=70

```

```

M(2)=608
GO TO 2
62 M(3)=772
M(2)=96
GO TO 2
63 M(4)=68
M(3)=768
M(2)=2
GO TO 2
64 M(4)=68
M(3)=2
M(2)=608
GO TO 2
65 M(4)=68
GO TO 47
66 M(4)=68
GO TO 49
67 M(4)=68
M(3)=2
M(2)=36
GO TO 2
68 M(4)=68
IF ( K-1 ) 1000,1068,54
1068 M(3)=578
GO TO 16
69 M(5)=576
GO TO 65
70 IF ( K-1 ) 1000,1070,2070
1070 M(5)=258
GO TO 43
2070 M(5)=1154
M(4)=576
M(3)=68
M(2)=1064
GO TO 2
71 M(4)=580
GO TO 47
72 M(4)=580
GO TO 55
73 M(4)=580
GO TO 61
74 M(4)=580
M(3)=2
M(2)=320
GO TO 2
75 M(2)=34
M(1)=49
GO TO 1
76 M(2)=546
M(1)=1043
GO TO 1
77 M(2)=34
M(1)=531
GO TO 1
78 M(1)=546
M(2)=1073
GO TO 1
79 M(3)=580
GO TO 75
80 M(3)=580

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      M(2)=34
      M(1)=1107
      G0 T0 1
81  M(2)=34
      M(1)=275
      G0 T0 1
82  M(3)=580
      G0 T0 81
83  M(3)=290
      G0 T0 75
84  M(3)=290
      G0 T0 77
85  IF ( K-1 ) 1000,1085,2085
1085 M(3)=324
      G0 T0 81
2085 M(3)=324
      M(2)=23
      G0 T0 2
86  IF ( K-1 ) 1000,1086,2086
1086 M(3)=836
      G0 T0 81
2086 M(3)=324
      M(2)=595
      G0 T0 2
87  M(4)=580
      G0 T0 83
88  M(4)=580
      IF ( K-1 ) 1000,1088,2088
1088 M(3)=1344
      G0 T0 81
2088 M(3)=1209
      M(2)=320
      G0 T0 2
89  M(3)=273
      G0 T0 75
90  M(3)=273
      M(2)=34
      M(1)=326
      G0 T0 1
91  M(3)=258
      G0 T0 76
92  M(3)=273
      M(2)=546
      M(1)=1350
      G0 T0 1
93  M(3)=258
      G0 T0 77
94  M(3)=273
      M(2)=34
      M(1)=838
      G0 T0 1
95  M(3)=258
      G0 T0 78
96  M(3)=1862
      M(2)=273
      M(1)=546
      G0 T0 1
97  M(4)=580
      G0 T0 89
98  M(4)=273

```

```

      G0 T0 80
99  M(3)=2
      G0 T0 75
100 M(3)=100
      G0 T0 75
101 M(3)=17
      G0 T0 77
102 M(3)=17
      M(2)=34
      M(1)=582
      G0 T0 1
103 M(3)=514
      G0 T0 75
104 M(3)=582
      G0 T0 75
105 M(3)=2
      G0 T0 77
106 M(3)=70
      G0 T0 77
107 M(4)=580
      G0 T0 99
108 M(4)=70
      G0 T0 79
109 M(4)=2
      G0 T0 80
110 M(4)=514
      G0 T0 80
111 M(3)=288
      G0 T0 81
112 M(3)=800
      G0 T0 81
113 M(3)=326
      G0 T0 81
114 M(3)=838
      G0 T0 81
115 M(3)=2
      G0 T0 81
116 M(3)=514
      G0 T0 81
117 M(3)=70
      G0 T0 81
118 M(3)=582
      G0 T0 81
119 M(4)=580
      G0 T0 115
120 M(4)=580
      G0 T0 116
121 M(4)=580
      G0 T0 111
122 M(4)=1346
      G0 T0 82
123 M(4)=256
      G0 T0 99
124 M(4)=256
      G0 T0 103
125 M(4)=85
      G0 T0 50
126 M(4)=597
      G0 T0 48
127 M(4)=256

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      G0 T0 100
128 M(4)=256
      G0 T0 104
129 M(4)=119
      G0 T0 85
130 M(4)=631
      G0 T0 85
131 M(4)=2
      G0 T0 84
132 M(4)=514
      G0 T0 84
133 M(4)=563
      IF ( K-1 ) 1000,86,50
134 M(4)=51
      G0 T0 48
135 M(4)=100
      G0 T0 84
136 M(4)=17
      G0 T0 58
137 M(4)=631
      IF ( K-1 ) 1000,86,59
138 M(4)=119
      IF ( K-1 ) 1000,86,56
139 M(5)=580
      G0 T0 123
140 M(5)=580
      G0 T0 127
141 M(5)=2
      IF ( K-1 ) 1000,88,2141
2141 M(4)=96
      M(3)=1689
      M(2)=580
      G0 T0 2
142 M(5)=514
      IF ( K-1 ) 1000,88,2142
2142 M(4)=1177
      M(3)=98
      M(2)=580
      G0 T0 2
143 M(1)=9394
      M(9) = 1067
      G0 T0 1
144 M(1)=11442
      M(9) = 5163
      G0 T0 1
145 M(1)=13490
      M(9) = 3115
      G0 T0 1
146 IF ( K-1 ) 1000,1146,2146
1146 M(1)=8868
      M(9)=330
      G0 T0 1
2146 M(2)=8192
      G0 T0 143
147 M(2)=290
      G0 T0 143
148 M(2)=290
      M(3)=290
      G0 T0 146
149 M(2)=307

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      GO TO 143
150 M(2)=273
      GO TO 143
151 M(2)=4403
      GO TO 144
152 M(2)=273
      GO TO 144
153 M(2)=2355
      GO TO 145
154 M(2)=273
      GO TO 145
155 IF ( K-1 ) 1000,1155,2155
1155 M(2)=307
      GO TO 1146
2155 M(3)=273
      GO TO 2146
156 M(2)=51
      GO TO 143
157 M(2)=17
      GO TO 143
158 M(2)=563
      GO TO 143
159 M(2)=529
      GO TO 143
160 IF ( K-1 ) 1000,1160,2160
1160 M(2)=17
      GO TO 1146
2160 M(3)=51
      GO TO 2146
161 IF ( K-1 ) 1000,1161,2161
1161 M(2)=597
      GO TO 1146
2161 M(3)=563
      GO TO 2146
162 M(3)=290
      GO TO 157
163 M(3)=290
      GO TO 159
164 M(3)=290
      GO TO 156
165 M(3)=290
      GO TO 158
166 M(3)=290
      M(4)=290
      GO TO 160
167 M(3)=290
      M(4)=290
      GO TO 161
168 M(2)=34
      GO TO 143
169 M(2)=546
      GO TO 144
170 M(2)=546
      GO TO 145
171 M(2)=34
      GO TO 145
172 M(2)=34
      GO TO 144
173 M(2)=546
      GO TO 143

```


174 M(2)=256
 GØ TØ 143
 175 M(3)=34
 GØ TØ 174
 176 M(3)=546
 GØ TØ 147
 177 M(5)=273
 GØ TØ 168
 178 M(3)=2321
 GØ TØ 169
 179 M(3)=4369
 GØ TØ 170
 180 M(3)=4369
 GØ TØ 171
 181 M(3)=2321
 GØ TØ 172
 182 M(3)=273
 GØ TØ 173
 183 M(3)=17
 GØ TØ 156
 184 M(3)=529
 GØ TØ 158
 185 M(5)=17
 GØ TØ 158
 186 M(3)=529
 GØ TØ 156
 187 M(3)=256
 GØ TØ 156
 188 M(3)=768
 GØ TØ 158
 189 M(3)=256
 GØ TØ 157
 190 M(3)=768
 GØ TØ 159
 191 M(4)=290
 GØ TØ 183
 192 M(4)=290
 GØ TØ 184
 193 M(4)=290
 GØ TØ 185
 194 M(4)=290
 GØ TØ 186
 195 M(3)=8868
 M(11)=330
 GØ TØ 16
 196 M(4)=68
 M(5)=516
 GØ TØ 195
 197 M(4)=580
 GØ TØ 195
 198 M(3)=8868
 M(11)=330
 GØ TØ 19
 199 M(4)=580
 GØ TØ 198
 200 M(4)=8868
 M(12)=330
 GØ TØ 47
 201 M(4)=8868
 M(12)=330

GO TO 48
 202 M(5)=68
 M(6)=516
 GO TO 200
 203 M(6)=8868
 M(14)=330
 GO TO 70
 204 M(5)=580
 GO TO 200
 205 M(4)=8868
 M(12)=330
 GO TO 61
 206 M(5)=580
 GO TO 205
 207 M(4)=19
 GO TO 195
 208 M(4)=887
 GO TO 195
 209 M(5)=68
 M(6)=516
 GO TO 207
 210 M(5)=68
 M(6)=516
 GO TO 212
 211 M(5)=580
 GO TO 207
 212 M(4)=1467
 GO TO 198
 213 M(4)=2047
 GO TO 198
 214 M(5)=580
 GO TO 213
 215 M(4)=8868
 M(12)=330
 GO TO 111
 216 M(5)=68
 M(6)=516
 GO TO 215
 217 M(5)=580
 GO TO 215
 218 M(4)=597
 GO TO 195
 219 M(1)=8868
 M(9)=330
 M(2)=34
 M(3)=529
 M(4)=68
 M(5)=516
 M(6)=258
 GO TO 1
 220 M(1)=834
 M(2)=580
 M(3)=356
 M(4)=1177
 M(5)=8868
 M(13)=330
 GO TO 1
 221 M(5)=17
 GO TO 200
 222 M(5)=597

```

      GO TO 201
223 M(5)=597
      GO TO 200
224 M(5)=17
      GO TO 201
225 M(7)=17
      GO TO 202
226 M(7)=529
      GO TO 202
227 M(7)=17
      GO TO 203
228 M(7)=529
      IF ( K-1 ) 1000,1228,203
1228 M(6)=1962
      GO TO 196
229 M(6)=580
      GO TO 221
230 M(6)=1177
      GO TO 206
1000 CALL EXIT
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

```

CELDIS FOR DISAGL

```

      SUBROUTINE CEL000
      COMMON M,L,X,Y,Z
      DIMENSION M(18),X(192),Y(192),Z(192)
      X(L-1) = MODF(X(L-1)+8.0,1.0)
      IF ( X(L-1)-.99999 ) 2,1,1
1 X(L-1) = 0.0
2 Y(L-1) = MODF(Y(L-1)+8.0,1.0)
      IF ( Y(L-1)-.99999 ) 4,3,3
3 Y(L-1) = 0.0
4 Z(L-1) = MODF(Z(L-1)+8.0,1.0)
      IF ( Z(L-1)-.99999 ) 6,5,5
5 Z(L-1) = 0.0
6 RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

```

```

CSYMDIS      SYMOPR FOR CORDIS
CSYMOPR      PROGRAM TO CONTROL SYMMETRY OPERATIONS
      SUBROUTINE SYMOPR
      COMMON NSPGRP,K,M,J,L,X,Y,Z,IX,IY,IZ,IHES,SX,SY,SZ
      DIMENSION X(192),Y(192),Z(192),IX(192),IY(192),IZ(192),IHES(192),
1 SX(192),SY(192),SZ(192),M(15)
8 FORMAT (32H0TWO ATOMS OCCUPY THE SAME SPACE/1H1)
      L=J+1
      L1=J
      DO 100 I =1,8
      IF ( M(I) ) 100,100,1
1 DO 99 L2=J,L1
      L3=L-1
      IF ( M(I)-8192 ) 4,5,4
5 X(L)=X(L2)+1.0/3.0
      Y(L)=Y(L2)+2.0/3.0
      Z(L)=Z(L2)+2.0/3.0
      IX(L) = IX(L2)
      IY(L) = IY(L2)
      IZ(L) = IZ(L2)
      SX(L) = SX(L2)
      SY(L) = SY(L2)
      SZ(L) = SZ(L2)
      IHES(L) = IHES(L2)
      X(L+1)=X(L2)+2.0/3.0
      Y(L+1)=Y(L2)+1.0/3.0
      Z(L+1)=Z(L2)+1.0/3.0
      IX(L+1) = IX(L2)
      IY(L+1) = IY(L2)
      IZ(L+1) = IZ(L2)
      SX(L+1) = SX(L2)
      SY(L+1) = SY(L2)
      SZ(L+1) = SZ(L2)
      L=L+1
      IHES(L) = IHES(L2)
      CALL CELOOO
      L=L+1
      CALL CELOOO
      GO TO 6
4 CALL OPERTR(I,L2)
6 L5=L
      L6=M(I)
7 L=L-1
      DO 90 L4=1,L3
      IF ( ABSF(X(L)-X(L4))-0.0001 ) 2,2,90
2 IF ( ABSF(Y(L)-Y(L4))-0.0001 ) 3,3,90
3 IF ( ABSF(Z(L)-Z(L4))-0.0001 ) 91,91,90
91 IF ( L4-J ) 92,93,93
92 PRINT 8
      STOP71634
93 CONTINUE
      L5=L3+1
90 CONTINUE
      IF ( L6-8192 ) 99, 98,98
98 L6=1
      GO TO 7
99 L=L5
      L1=L-1
100 CONTINUE
101 J=L
      RETURN
      END

```

*	FAP	
	LBL	OPERTR,A
	ENTRY	OPERTR
OPERTR	CLA*	1,4
	SXA	EXIT,4
	SXA	EXIT+1,2
	SXA	EXIT+2,1
	PDX	,1
	CLA*	2,4
	PDX	,2
	LXD	L,4
	CLA	M+1,1
	ARS	18
	PAI	
	RFT	20000
	TRA	TRIPLE
	CLA	IHEX+1,2
	STO	IHEX+1,4
	CLA	X+1,2
	RFT	1
	CLA	Y+1,2
	RFT	2
	CHS	
	RFT	4
	FAD	H
	RFT	10
	FAC	H+1
	STO	X+1,4
	CLA	Y+1,2
	RFT	20
	CLA	X+1,2
	RFT	40
	CHS	
	RFT	100
	FAD	H
	RFT	200
	FAD	H+1
	STO	Y+1,4
	CLA	Z+1,2
	RFT	400
	CHS	
	RFT	1000
	FAD	H
	RFT	2000
	FAD	H+1
	RFT	4000
	FAD	H+2
	RFT	10000
	FAD	H+3
	STO	Z+1,4
	RNT	1
	TRA	IHXO
	CLS	IHEX+1,4
	TZE	IHXO
	ADD	=03000000
	STO	IHEX+1,4
IHXO	CLA	B11+1,2
	RFT	1
	CLA	B22+1,2
	STO	B11+1,4

	CLA	B22+1,2
	RFT	20
	CLA	B11+1,2
	STO	B22+1,4
	CLA	B33+1,2
	STO	B33+1,4
	CLA	SX+1,2
	RFT	1
	CLA	SY+1,2
	RFT	2
	CHS	
	STO	SX+1,4
	CLA	SY+1,2
	RFT	20
	CLA	SX+1,2
	RFT	40
	CHS	
	STO	SY+1,4
	CLA	SZ+1,2
	RFT	400
	CHS	
	STO	SZ+1,4
	TXI	*+1,4,1
	SXD	L,4
	CALL	CELO00
EXIT	AXT	,4
	AXT	,2
	AXT	,1
	TRA	3,4
TRIPLE	CLA	H+4
	RFT	1
	CLA	X+1,2
	RFT	2
	FSB	Y+1,2
	RFT	4
	CLA	Z+1,2
	RFT	10
	CHS	
	STU	X+1,4
	CLA	H+4
	RFT	20
	CLA	Y+1,2
	RFT	40
	FSB	X+1,2
	RFT	100
	CLA	Z+1,2
	RFT	200
	CHS	
	STO	Y+1,4
	RFT	400
	CLA	X+1,2
	RFT	1000
	CLA	Y+1,2
	RFT	2000
	CLA	Z+1,2
	RFT	4000
	FAC	H+2
	RFT	10000
	FAC	H+3

	STG	Z+1,4
	RNT	3
	TRA	TR1
	CLA	=C2000000
	TRA	TR4
TR1	RNT	60
	TRA	TR2
	CLA	=C1000000
TR4	STO	IHEX+1,4
	CLA	B11+1,2
	STG	B11+1,4
	CLA	B22+1,2
	STG	B22+1,4
	CLA	SX+1,2
	STG	SX+1,4
	CLA	SY+1,2
	STG	SY+1,4
	TRA	TR3
TR2	RFT	1
	CLA	B11+1,2
	RFT	2
	CLA	B22+1,2
	RFT	4
	CLA	B33+1,2
	STG	B11+1,4
	RFT	20
	CLA	B22+1,2
	RFT	40
	CLA	B11+1,2
	RFT	100
	CLA	B33+1,2
	STG	B22+1,4
	RFT	1
	CLA	SX+1,2
	RFT	2
	CLA	SY+1,2
	RFT	4
	CLA	SZ+1,2
	STG	SX+1,4
	RFT	20
	CLA	SY+1,2
	RFT	40
	CLA	SX+1,2
	RFT	100
	CLA	SZ+1,2
	STG	SY+1,4
	RFT	400
	CLA	B11+1,2
	RFT	1000
	CLA	B22+1,2
	RFT	2000
TR3	CLA	B33+1,2
	STG	B33+1,4
	RFT	400
	CLA	SX+1,2
	RFT	1000
	CLA	SY+1,2
	RFT	2000
	CLA	SZ+1,2
	STG	SZ+1,4

	TXI	**+1,4,1
	SXD	L,4
	SXA	**+2,4
	CALL	CELO00
	AXT	,4
	RNT	20000
	TRA	EXIT
	CLA	M-7,1
	ARS	18
	PAI	
	TRA	TRIPLE
H	DEC	0.5,0.25,0.33333333,0.66666667,0.0
NSPGRP	COMMON	1
K	COMMON	1
M	COMMON	15
J	COMMON	1
L	COMMON	1
X	COMMON	192
Y	COMMON	192
Z	COMMON	192
B11	COMMON	192
B22	COMMON	192
B33	COMMON	192
IHEX	COMMON	192
SX	COMMON	192
SY	COMMON	192
SZ	COMMON	192
	END	