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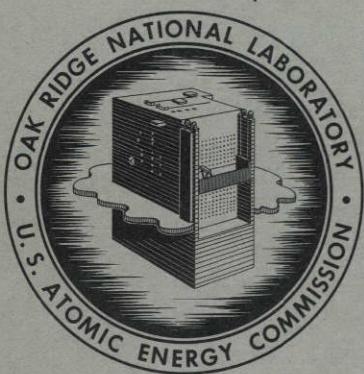
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OR TEP:

A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM
FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Carroll K. Johnson



OAK RIDGE NATIONAL LABORATORY
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

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CHEMISTRY DIVISION

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JUNE 1965

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OR TEP: A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

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ABSTRACT

This report describes a computer program for drawing crystal structure illustrations with a mechanical plotter. Ball-and-stick type illustrations of a quality suitable for publication are produced with either spheres or thermal-motion probability ellipsoids on the atomic sites. The program can produce stereoscopic pairs of illustrations which aid in the visualization of complex packing arrangements of atoms and thermal motion patterns. Interatomic distances, bond angles, and principal axes of thermal motion are also calculated to aid the structural study.

The FORTRAN coding utilizes the comparable features of IBM 709/7090 FORTRAN II and CDC 1604/1604A FORTRAN 63 so that the program can be executed on a number of different machines which have 32 K word memories. The machine-oriented plotting subroutines are standard library-type routines with slight modifications. Both CalComp and Benson Lehner off-line magnetic-tape plotting systems have been used successfully.

Sample stereo-figure illustrations and a viewer are included with the report.

1. INTRODUCTION

Appropriate illustrations are essential in any manuscript dealing with crystallographic structures. An often quoted expression might justifiably be paraphrased to read that a well-planned figure is worth a thousand numbers. With the so-called information explosion in its early exponential stages, the author of a structure paper should feel particularly obligated to help the reader as much as he can with "crystal clear" illustrations.

This computer program, OR TEP (Oak Ridge Thermal Ellipsoid Plot program) is an attempt to supply a tool which can reduce the tedium associated with drawing certain types of crystal structure illustrations. In addition, the precision obtainable through machine plotting makes feasible the production of detailed stereoscopic illustrations which are impractical to draw by conventional drafting methods. The program does not in any sense replace the experience of the crystallographic draftsman; it is only a way of implementing certain of his ideas. Touching up the figures by hand to correct for overlap and to add further detail greatly enhances the figure's appeal and usefulness. The user is encouraged to do this and not to be content with the raw illustrations as they come from the plotter.

Four major goals were specified for OR TEP, and they are listed here in the order of their assigned importance. (1) The program must produce high quality illustrations, including stereoscopic pairs of thermal-motion figures, as free as possible of visually distracting approximations. (2) The program must be general both with respect to the types of illustrations it can draw and the types of computing and plotting equipment that it can utilize. (3) The program must be easy to use and require a minimum of input; it should also be easy to modify. (4) The computation time should be minimized. Memory size limitation was not one of the considerations; hence the program requires a 32 K word memory.

Stereoscopic crystal structure illustrations were used quite extensively in the 1920's and 1930's, particularly by M. von Laue and R. von Mises in their beautifully done two-volume series of stereoscopic drawings.¹ More recently, computer techniques were applied in making crystal structure stereoscopic pictures by W. R. Busing² using an IBM 704 computer with cathode ray tube output. The availability of larger, faster computers and higher resolution plotting devices led quite naturally to the present work. As usual, there is an unlimited horizon for future work with more sophisticated ideas and equipment.

I am particularly indebted to my colleagues, Drs. H. A. Levy, W. R. Busing, G. M. Brown, and R. D. Ellison, for many helpful discussions, and to R. A. Hollister, a summer participant with the ORNL Mathematics Division, who helped plan and code several parts of the program. The initial version of OR TEP was written as a subroutine for the Busing, Martin, and Levy Function and Error Program, OR FFE;³ and many of the concepts and several of the subroutines of OR FFE are incorporated into the present program. Several parts of EIGEN were taken from a program written by R. E. Funderlic and B. Franz from the Central Data Processing group. Subroutine AXEQB was adapted from a subroutine obtained from the Oak Ridge Central Data Processing Library.

This report covers the following topics. First, Sect. 2.1 is a summary table of instructions and is the part of the report to which the experienced user will routinely refer. Next, the philosophy of the program is outlined and an example given. Section 3 defines the terms used in this report and describes the input in detail. The computational procedures used by the program are discussed in Sect. 4, and steps are outlined for adapting the program to other configurations of equipment. The next section summarizes the mathematics of thermal motion probability ellipsoids. Section 6 contains a number of examples of figures produced with OR TEP. Most of these drawings are stereoscopic pairs of perspective projections and are included to illustrate the information transfer advantages gained through the use of stereo figures. The final section contains the complete OR TEP FORTRAN listing.

2. GENERAL PRINCIPLES AND PROCEDURES

2.1 Summary Table of Instructions

A brief summary of the input cards is given at this point to serve as a check list for use with OR TEP. All aspects are explained in detail in Sect. 3.

1. *Title card* (see 3.2.1)
2. *Cell parameter card* (see 3.2.2)
3. *Symmetry cards* with sentinel in column 1 on last card (see 3.2.3)
4. *Atomic parameter cards* (two per atom) with sentinel in column 1 of very last card (see 3.2.4)
5. *Instruction cards* with -1 in columns 8 and 9 of final instruction card. The instructions are summarized in Table 2.1 and explained in detail in Sect. 3.3.

¹M. von Laue and R. von Mises (eds.), *Stereoscopic Drawings of Crystal Structures*, vols. I and II, Springer, Berlin, 1926 and 1936.

²W. R. Busing, *Abstract of Washington, D. C., Meeting of the ACA, Jan. 24-27, 1960*, F-7, p. 23.

³W. R. Busing, K. O. Martin, and H. A. Levy, *OR FFE, a FORTRAN Crystallographic Function and Error Program*, ORNL-TM-306 (March 1964).

Table 2.1. Summary Table of All Instructions

Function	1-3	4-9	10-18	19-27	28-36	37-45	46-54	55-63	64-72
Structure analysis									
Distances	0 or 2	101	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	-	-
Dist. + ang.	0 or 2	102	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	-	-
Princ. axes	-	103	-	-	-	-	-	-	-
Plotter control									
Initialize	-	201	-	-	-	-	-	-	-
Advance and term.	-	202	X(IN)	Y(IN)	-	-	-	-	-
Plot boundary									
Dimensions	-	301	X(IN)	Y(IN)	VIEW(IN)	BRDR(IN)	-	-	-
Title rotation	-	302	THETA ($^{\circ}$)	-	-	-	-	-	-
Retrace displace	-	303	X(IN)	-	-	-	-	-	-
Atoms list									
Run add	-	401	From	(-) to	From	(-) to
Run subtract	-	411	From	(-) to	From	(-) to
Sphere add	0 or 2	402	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	-	-
Sphere subtract	0 or 2	412	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	-	-
Box add	-	403	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Box subtract	-	413	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Zero atoms list	-	410	-	-	-	-	-	-	-
Cartesian system									
Definition	-	501	ORG N	V1A	V1B	V2A	V2B	-	-
Rotate reference	-	502	Axes No.	Rotate ($^{\circ}$)	Axes No.	Rotate ($^{\circ}$)
Rotate working	-	503	Axes No.	Rotate ($^{\circ}$)	-	-	-	-	-

Table 2.1 (continued)

Function	1-3	4-9	10-18	19-27	28-36	37-45	46-54	55-63	64-72
Center and scale									
Explicit	-	601	XO (IN)	YO (IN)	SCAL1	SCAL2	-	-	-
Scale only	-	602	XO (IN)	YO (IN)	-	SCAL2	-	-	-
Center only	-	603	-	-	SCAL1	SCAL2	-	-	-
Center and scale	-	604	-	-	-	SCAL2	-	-	-
I. P. and I. S. ^a	-	611	ΔXO (IN)	ΔYO (IN)	ΔSCAL1	SCAL2	-	-	-
I. P. and scale	-	612	ΔXO (IN)	ΔYO (IN)	-	SCAL2	-	-	-
I. S. and center	-	613	-	-	ΔSCAL1	SCAL2	-	-	-
Ellipsoids									
Shaded football	0 or 1	701	-	-	-	-	SYM HGT	PAR-OFF ^b	PER-OFF ^c
(Format No. 1 trailer card)	-	-	A0 (IN)	A1 (IN)	-	-	-	-	-
Football	0 or 1	702	(same as 701)						
Open model	0 or 1	703	(same as 701)						
Boundary only	0 or 1	704	(same as 701)						
Other types	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	SYM HGT	PAR-OFF ^b	PER-OFF ^c
(Format No. 1 trailer card)	-	-	A0 (IN)	A1 (IN)					
As above except no printed output of individual coordinates	0 or 1	711	(same as 701)						
0 or 1	712	(same as 701)							
0 or 1	713	(same as 701)							
0 or 1	714	(same as 701)							
0 or 1	715	(same as 705)							
Bonds									
Explicit (cont.)	0 or 1	801	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)
Implicit fancy	2	802	-	-	-	-	-	-	-
(Format No. 2 trailer card)									
Implicit line	2	803	-	-	-	-	-	-	-
(Format No. 2 trailer card)									

^aI. P. and I. S. signifies increment position and increment scale.^bPAR-OFF signifies parallel offset (in.).^cPER-OFF signifies perpendicular offset (in.).

Table 2.1 (continued)

Function	1-3	4-9	10-18	19-27	28-36	37-45	46-54	55-63	64-72
As above except no printed output	—	811	(same as 801)						
	2	812	(same as 802)						
	2	813	(same as 803)						
Labels									
CHEM SYMB	—	901	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
REG TITLES	3	902	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3 title card									
PROJ VECT TITLE	3	903	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3 title card									
VECTOR TITLE	3	913	ATOM-1	ATOM-2	—	—	HGT (IN)	PAR-OFF	PER-OFF
Format No. 3 title card									
PROJ BOND LABEL (1, 2, 3 dec. places)	—	904	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
	—	905							
	—	906							
BOND LABEL (1, 2, 3 dec. places)	—	914	ATOM-1	ATOM-2	—	—	HGT (IN)	PAR-OFF	PER-OFF
	—	915							
	—	916							
CENTERED SYMB		908	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(with pen up or pen down)	1	909							
(Format No. 1 trailer card)	1	—	SYMB#	—	—	—	—	—	—
Saved sequence	—								
START	—	1101	—	—	—	—	—	—	—
STOP	—	1102	—	—	—	—	—	—	—
EXECUTE	—	1103	—	—	—	—	—	—	—
Terminate job	—	—1	—	—	—	—	—	—	—
New job follows (from title card on)	—	—2	—	—	—	—	—	—	—

2.2 Programming a Nonstereoscopic Illustration for OR TEP

2.2.1 General Comments on Automated Graphics. — In order to produce high quality illustrations with OR TEP, one must in general use an iterative approach; that is, the illustration must usually be computed and plotted several times before an optimal figure is produced. With each trial, as many factors as possible are optimized to give a more informative and more esthetically pleasing result. One often requires about four trials for a stereoscopic figure of an unfamiliar structure (barring blunders and plotter malfunctions).

Overlap is one of the major problems, particularly for chemical symbols and bond distance labels. If the user is not drawing stereoscopic figures, it is often better to do the lettering with a LeRoy lettering template instead of the computer. The template lettering is neater than the computer lettering, and it can be positioned much more easily. However, for stereoscopic lettering the manual procedure appears to be unsatisfactory because of the necessity for exact relative placement of the lettering on the two views to maintain good stereopsis.

Overlapping atoms are another problem. The program does not leave out the parts of an atom hidden behind other atoms. This feature would be a difficult (although not impossible) programming feat. This can be accomplished manually, however, by erasing or "whiting out" the unwanted parts of an atom. Even with stereo views, the figures are more effective if overlap is taken care of, especially when "opaque" ellipsoids are used.

In order to maintain generality in OR TEP, the concept of programming is applied to the problem of drawing illustrations with a plotter. This concept allows access to a series of basic building block operations which are put together by the user to "program" an illustration. The instructions used in programming OR TEP are divided into the following categories: (1) instructions used to specify preliminary graphical details, (2) instructions used to compose an illustration, (3) instructions used to draw the illustration, (4) instructions used to repeat a sequence of other instructions, and (5) termination instructions. Each instruction starts on a separate punched card and contains an identifying number and whatever parameters are needed for the particular instruction. The general role of these instructions is explained in the remaining sections of Part 2, and the individual instructions are described in detail in 3.3. The simplest way to construct the program is, first, to scan through the list of instructions in numerical order and pick out the relevant ones to construct the framework of the program. Then certain other instructions are placed into the framework program to furnish the remaining "bookkeeping" details.

Let us assume that the structural data cards (described in 3.2) have been prepared for a crystal structure and that we want to prepare a program to draw a single nonstereographic figure of the contents of one unit cell. We describe next the general stepwise procedure one would follow to program such an illustration.

2.2.2 Preliminary Graphical Details. — The first instruction card should be the plotter control instruction 201 (see 3.3.3.1) which will initialize the plotting package.

Next, the plot boundary instruction 301 (see 3.3.4.1) is needed to set the following parameters: (1) X dimension in inches for the plot boundary, (2) Y dimension in inches for the plot boundary, (3) viewing

distance in inches for perspective projection (zero as a signal for parallel projection), and (4) border (or margin) dimension inside the boundary.

No other 200 or 300 series instructions are required for this particular hypothetical figure.

The preliminary graphical details are analogous to what a draftsman might do in setting up his drafting board in preparation for a drawing.

2.2.3 Composing the Illustration. — This step involves specifying: (1) which atoms are to be used as the figure subject, (2) the rotational orientation of the subject, and (3) the scaling and positioning of the subject relative to the drawing area. These three components of composition are implemented by the 400, 500, and 600 series instructions respectively.

For our hypothetical example, suppose we want to place the *b* crystal axis along the plotter *x* axis and the *c* axis of the crystal in the plotter *xy* plane as nearly as possible parallel to the plotter *y* axis. This setting can be accomplished with a 501 instruction (see 3.3.6.1) alone; but if additional reorientation were necessary, a 502 instruction (see 3.3.6.2) would also be used.

A rectangular box of enclosure can be described with a 403 instruction (see 3.3.5.3) to contain the desired atoms for the subject definition. The scaling and positioning of the subject to fill the drawing area may be accomplished automatically with a 604 instruction (see 3.3.7.1).

2.2.4 Drawing the Illustration. — Crystal structure illustrations of the ball-and-stick type are made up of three components: balls (atoms), sticks (bonds), and labels. The three components are drawn with the 700, 800, and 900 instruction series respectively; the first two instruction series can also perform certain types of labeling.

The atom representation can be either a general ellipsoid or a boundary ellipse. In some cases these become a sphere and a circle. Chemical symbols may be plotted simultaneously with the atoms.

For our example we might simply draw circles and put the chemical symbols within the circles by using instruction 704 (see 3.3.8.1). This instruction will draw all the atoms of the subject and their chemical symbols.

The bonds are not always necessary in a drawing, but for structures with molecules or with distinctive groupings they are usually quite helpful. The most convenient method for describing and drawing bonds is instruction 812 (see 3.3.9.2). This instruction uses vector search codes (see 3.1.5) which reflect the user's knowledge of the structural chemistry and the interatomic distance ranges for the compound being drawn. Covalent bonds or any other desired type are found and drawn automatically from the list of atoms which make up the subject. If desired, the interatomic distance label can also be drawn with each bond (see 3.3.9).

Various types of labeling can be done with the 900 series instruction. The one which will most often be included is a caption for the figure using instruction 902 (see 3.3.10.2).

2.2.5 Terminating the Drawing of the Illustration. — The plotter control instruction 202 (see 3.3.3.2) allows the user to remove the finished drawing from the plotting area and to place a fresh area of plot paper in position for any additional plots which may be drawn.

To terminate the computer job, a (-1) instruction (see 3.3.12) would be used as the last instruction of the program.

2.3 Programming a Stereoscopic Illustration for OR TEP

A stereoscopic pair of figures is simply two perspective views of the subject as seen from two different viewpoints (which are usually about 6° apart). This pair is produced with OR TEP by programming for two drawings. A few additional instructions supplementary to those outlined in 2.2 are useful for producing stereo figures. These instructions are the stereoscopic rotation instruction 503 and the 1100 series of instructions, which facilitate the repetition of a series of instructions.

2.3.1 Stereoscopic Rotations. — In general, one member of a detailed stereoscopic illustration cannot be drawn completely independent of the other member of the pair because certain features (e.g., which octant of an ellipsoid is shaded) must be done identically in the two drawings. In OR TEP the "stereoscopically sensitive decisions" are handled by using two Cartesian coordinate systems: the reference Cartesian system and the working Cartesian system (see 3.1.8). The steps involved in picture composition (see 2.2.3) and the stereoscopically sensitive decisions are always based on the reference system, but the drawing of the illustration (see 2.2.4) is always based on the working system. A stereoscopic rotation is simply a rotation of the working system *from the reference system* about the axis which is vertical while viewing the final result. For example, a nominal rotation of $+3^\circ$ about the plotter *y* axis might be used for the left-eye view and a rotation of -3° about the same axis might be made before plotting the right-eye view, thus producing a total interocular angle of 6° .

A program to draw a stereo pair would involve the following steps:

1. preliminary graphical details,
2. composition of subject,
3. left-eye stereo rotation,
4. draw the subject,
5. advance the plotter,
6. right-eye stereo rotation,
7. draw the subject,
8. advance the plotter,
9. terminate the job.

2.3.2 Repeating a Sequence of Operations. — It should be noted that steps 7 and 8 in the stereo program of the last section are identical to steps 4 and 5. The program can be shortened somewhat by using the "saved sequence" instructions (see 3.3.11). A 1101 instruction (start saved sequence) would be placed between 3 and 4, and a 1102 instruction (end saved sequence) between 5 and 6. Then steps 7 and 8 can be replaced by a 1103 instruction (execute saved sequence).

Any sequence of instructions can be saved in this manner and repeated as many times as desired with 1103 instructions. For example, the saved sequence feature can be used to produce a complete series of views of a structure at (say) 15° intervals about an axis. Note that the instructions between the start and stop instructions are *both executed and saved* the first time through.

2.4 Drawing the Cubane Structure: An Example

The novel compound cubane⁴ (C_8H_8) has been crystallized and the structure determined.⁵ The carbon-carbon bonds lie along the edges of a cube within experimental error. The compound crystallizes with the trigonal symmetry of space group $\bar{R}\bar{3}$. One carbon and one hydrogen are in special positions along the $\bar{3}$ axis, and the remaining carbon and hydrogen are in general positions. Anisotropic temperature factor coefficients were fitted to the carbon atoms during the least-squares refinement of the structure, and isotropic temperature factors were used for the hydrogen atoms.

The cell parameters are

$$a = b = c = 5.34 \text{ \AA} ,$$

$$\alpha = \beta = \gamma = 72.26^\circ .$$

The equivalent positions of space group⁶ $\bar{R}\bar{3}$ are $x, y, z; z, x, y; y, z, x; \bar{x}, \bar{y}, \bar{z}; \bar{z}, \bar{x}, \bar{y};$ and $\bar{y}, \bar{z}, \bar{x}.$

The positional parameters for C1, C2, H1, and H2 are given as -0.18711, 0.19519, 0.10706; 0.11546, 0.11546, 0.11546; -0.3246, 0.3468, 0.1848; and 0.2100, 0.2100, 0.2100, respectively. The anisotropic temperature factors given for the carbon atoms are of the type called zero⁷ in this report (see 3.2.4.2). The coefficients $b_{11}, b_{22}, b_{33}, b_{12}, b_{13}, b_{23}$ for C1 and C2 are 0.0410, 0.0425, 0.0450, -0.0042, -0.0142, -0.0051; and 0.0468, 0.0468, 0.0468, -0.0143, -0.0143, -0.0143.

2.4.1 Data Input for Cubane. — 2.4.1.1 Title Card (see 3.2.1). — FORMAT (12A6)

Card No.

(1) CUBANE (E. B. FLEISCHER (1964) J. A. C. S. 86, 3889)

2.4.1.2 Cell Parameter Card (see 3.2.2). — FORMAT (6F9.6)

(2)	5.34	5.34	5.34	72.26	72.26	72.26
-----	------	------	------	-------	-------	-------

2.4.1.3 Symmetry Cards (see 3.3.3)

FORMAT (I1, F14.10, 3F3.0, 2(F15.10, 3F3.0))

(3)	0	0.	1	0	0	0.	0	1	0	0.	0	0	1
(4)	0	0.	0	0	1	0.	1	0	0	0.	0	1	0

⁴P. Eaton and T. Cole, *J. Am. Chem. Soc.* **86**, 3157 (1964).

⁵E. B. Fleischer, *J. Am. Chem. Soc.* **86**, 3889 (1964).

⁶N. F. M. Henry and K. Lonsdale (eds.), *International Tables for X-Ray Crystallography*, vol. I, Kynoch, Birmingham, 1962.

⁷Unfortunately, many authors of structure papers neglect to define the equation for the anisotropic temperature factor coefficients. In the present case, the type can be determined from the comparative isotropic temperature factor listed in anisotropic form in their Table I. In other instances one must arbitrarily choose a type (usually 0, 1, or 4 in the U.S.A.) and do the principal axis transformation, then check that the principal values are correct, or at least reasonable. In particular, the principal values must all be positive.

Card No.

(5)	0	0. 0 1 0	0. 0 0 1	0. 1 0 0
(6)	0	0. -1 0 0	0. 0 -1 0	0. 0 0 -1
(7)	0	0. 0 0 -1	0. -1 0 0	0. 0 -1 0
(8)	1	0. 0 -1 0	0. 0 0 -1	0. -1 0 0

2.4.1.4 Atomic Parameter Cards. -

Positional parameters (see 3.3.4.1): FORMAT (A6, 3X,5F9.6,F9.0)

Thermal parameters (see 3.2.4.2): FORMAT (I1, F8.6,5F9.6,F9.0)

Atoms 1 and 2 are entered with positional parameters type 0 and anisotropic temperature factors type 0.

Card No.

(9)	C1			-.18711	.19519	.10706	0	
(10)	0	.04100	.04250	.04500	-.00420	-.01420	-.00510	0
(11)	C2				.11546	.11546	.11546	0
(12)	0	.04680	.04680	.04680	-.01430	-.01430	-.01430	0

Atoms 3 and 4 are entered with positional parameters type 0 and with dummy sphere temperature factors (type 7) 0.1 Å in radius.

(13)	H1			-.32460	.34680	.18480	0
(14)	0	.1					7
(15)	H2			.21000	.21000	.21000	0
(16)	0	.1					7

Atom 5 is a dummy atom at the cell origin with a blank card dummy sphere (see last paragraph of 3.2.4.2). This could also be entered with type 7 as were atoms 3 and 4.

(17)	ORGN			.00000	.00000	.00000	0
(18)	1						0

In the card deck for this sample program, extensive use of Format No. 3 trailer cards (see 3.3.1) is made as a method of including a comment with an instruction. This convention is not mandatory, but it is a convenient method for annotating a program. This example uses a wide range of instructions in order to demonstrate them. As in the case with any programming system, there are many ways of doing any given problem. The Formats are described in 3.3.

2.4.2 Analysis of Structure (see 3.3.2). — These instructions are not connected with producing the figure. They are shown here just to demonstrate how they are used. A 101 instruction is used to obtain a tabulation of the atoms surrounding one atom or a series of several designated atoms. To obtain a list of all atoms (hydrogen and carbon atoms) out to a limit of (say) 3.61 Å about the two carbons C1 and C2, one would use the following instruction. (The notation is explained in Section 3.3.2.)

Card No.

(19) 101 155501 2 1 4 3.61

Atoms 1 through 2 of Atoms 1 through 4 of all symmetry *D* max
symmetry operation 1 and translation operations

A 102 instruction gives both interatomic distances and interatomic angles. In order to find all covalent bonds and bond angles about the two carbons we might use the following instruction.

(20) 102 155501 2 1 4 1.8

In this case a smaller *D* max was used so that only the distances and angles of immediate interest would be computed.

2.4.3 Programming the Cubane Illustration. — First we must initialize the plotter package.

(21) 201

The two plot boundary dimensions can be equal for the present illustration since the cubane molecule is a cube. Suppose we use an 11- by 11-in. boundary and specify a 1-in. margin to give a total working area of 9 by 9 in. A 24-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 24 1

In general we would use retracing to make the lettering, and certain other details, stand out more prominently. However, for the test example we will eliminate the retracing so that the illustration will plot as fast as possible.

(23) 303 0

The subject of the illustration is a single cubane molecule, which we will now define. One way of designating this subject is to specify a sphere of enclosure, centered on the dummy atom 555501, which is at the center of a cubane molecule. A radius of 3.2 Å should be adequate to isolate a single molecule.

Card No.

(24)	402	<u>555501</u>	5	<u>1</u>	<u>4</u>	<u>3.2</u>
		(a)		(b)		(c)

where the several parts designate:

- (a) a run of origin atom (center of sphere) from atom 5 to atom 5 in symmetry position 55501 (that is, in this example, a single sphere),
- (b) a run of target atom from atom 1 to atom 4, and
- (c) a sphere radius of 3.2 Å.

To orient the molecule, we will first define a coordinate system along the edges of the cubane cube. We will then rotate the molecule relative to this coordinate system to minimize overlap.

The origin of the coordinate system will be positioned on the dummy atom No. 5. The desired coordinate system orientation will be defined by specifying two vectors from the special position atom 255501 to the two symmetry-related general-position atoms 155501 and 155502.

(25)	501	555501	255501	155501	255501	155502	0	0
------	-----	--------	--------	--------	--------	--------	---	---

A rotation of 25° about the Y axis (axis 2) followed by a rotation of 28° about the X axis (axis 1) will produce a satisfactory view of the molecule.

(26)	502	2	25	1	28
------	-----	---	----	---	----

The stereoscopic rotation for the left eye can be done at this point just to keep the instructions in numerical order. We will use a rotation of 3° about the Y axis (axis 2) for the left-eye view. Later in the program, we will make a -3° rotation about the same axis for the right-eye view to give a total interocular angle of 6°.

(27)	503	2	3.0	
------	-----	---	-----	--

To scale and position the subject for projection onto the drawing board, we will use two instructions. The first will automatically scale and position the subject to utilize all available space. The second will shrink the scale slightly to allow more space along the border.

A 604 instruction will automatically set X0, Y0, and SCAL1. However, the ellipsoid scale factor ratio SCAL2 must be specified independently. If we want thermal ellipsoids corresponding to 50% probability, then we will enter 1.54 for SCAL2.

(28)	604	0	0	0	1.54
------	-----	---	---	---	------

To shrink the overall scale factor (SCAL1) by 10% we use the incremental instruction 611 and enter 0.9 for SCAL1.

Card No.

(29) 611 0 0 .9 0

This completes the composition of the illustration.

Since the structure will be drawn twice, once for each eye, the "saved sequence" feature can be used to shorten the program. Note that the instructions between the start and stop instructions are both *executed and saved* the first time through. They can then be re-executed as many times as desired by using the "execute saved sequence" instruction 1103.

The 1101 instruction starts the saved sequence.

(30) 1101

The ATOMS list currently contains all the atom designators for one cubane molecule. We want to draw the molecule in two separate steps so that the hydrogen and carbon atoms can be given different graphical representations. To eliminate the hydrogens from the list we use a sphere-of-enclosure elimination instruction and include only the hydrogens in its target list. This will leave only the carbon atom designators in the atoms list.

(31) 412 555501 5 3 4 3.2

To draw the carbon atoms we will construct a special code that (a) draws the three principal-plane forward traces and the boundary-plane trace (NPLANE = 4), (b) omits the reverse sides of the principal planes (NDOT = 0), (c) draws the forward principal axes without additional shading (NLINE = 1), and (d) omits the reverse principal axes (NDASH = 0). In addition we want the chemical symbols to be drawn with letters 0.2 in. high (before projection) and displaced from the atomic center by 0.6 in. in the horizontal direction and 0.7 in. in the vertical direction.

(32) 715 4 0 1 0 .2 .6 .7

The 715 instruction is used, rather than 705, to shorten the output listing of the example. Normally we would use the 705 to obtain a listing of all coordinates.

To draw the hydrogen atoms we must first clear the atoms array.

(33) 410

We then rebuild it with hydrogen atom designators alone. We could use a sphere of enclosure; however, for variety we will use an atom designator code run instead. The atom numbers run from 3 through 4 and the symmetry operators run from 1 through 6. All atoms will be in cell 555; consequently, there are no translation runs. Since one of the atoms (atom 4) is in a special position, duplicate entries will occur; but they are eliminated automatically.

Card No.

(34) 401 355501 - 455506

Since the hydrogen atoms are to be drawn with a standard model, the construction details will be taken care of automatically. We want chemical symbols 0.2 in. high and offset 0.35 in. horizontally and 0.4 in. vertically.

(35) 712 0 0 0 0 .2 .35 .4

Before drawing the bonds, we must reconstruct the complete molecule. This can be accomplished with a sphere of enclosure identical to the original one. The hydrogens that are already in the atoms list will not cause complications, since duplicates are automatically eliminated.

(36) 402 555501 5 1 4 3.2

The most convenient procedure for drawing bonds is to use the implicit bond instruction 812. All other information can be entered with a single format No. 2 trailer card (vector search code card).

(37) 2 812

(38) 0 $\frac{1}{(a)} \frac{4}{(b)}$ $\frac{1}{(c)} \frac{4}{(d)}$ $\frac{4}{(e)}$ $\frac{.9}{(d)} \frac{1.6}{(e)}$

where

- (a) and (b) are atom number runs for atom-pair bonds to be drawn,
- (c) denotes bond type 4,
- (d) denotes the distance range 0.9 to 1.6 Å, which will cover all covalent bond distances, and
- (e) the bond radius, is 0.04 Å.

The remaining fields in the card can be blank, since a complete set of bond distance labels is not desired.

Because of the symmetry, there are only two different C-C bond lengths in cubane. These are C1-C1 and C1-C2. We shall label one example of each of these bonds. For variety let us label one with a normal bond-length label and the other with a perspective label. The two bonds which can be labeled most advantageously are (a) 155504 → 155503 and (b) 255504 → 155505. The labels will be 0.15 in. in height and displaced vertically from the bond center by -0.4 in.

(39) 906 155504 155503 0 0 .15 0 -.4

(40) 916 255504 155505 0 0 .15 0 -.4

The final feature to be drawn is a caption (CUBANE) for the illustration. This can conveniently be positioned by "hanging" it from the dummy atom 555501 and "bouncing" it 1 in. off the lower y boundary.

Card No.

(41) 3 902 555501 0 0 1. .25 0 0

(42) CUBANE

The saved sequence can now be terminated.

(43) 1102

The plotter is then advanced 9 in. along x in preparation for the right-eye view.

(44) 202 9

The stereo rotation of -3° about axis 2 is now performed in preparation for the right-eye view. (Note that this rotation starts with the reference orientation, not the previous working orientation.)

(45) 503 2 -3.0

The saved sequence can now be repeated for the right eye. Note that the atom list now contains the same information that it did when the first view was drawn.

(46) 1103

The illustration is now complete. The plotter is next advanced 20 in. along x to remove this figure from the working area.

(47) 202 20

A dummy plot for the CalComp system is now added to aid in stopping the CalComp plotter.

(48) 202 0

Finally we terminate the job and exit from the program.

(49) -1

2.4.4 Stereoscopic Illustration of Cubane. — Figure 2.1 shows the stereoscopic pair exactly as it was plotted by the CalComp 580 system. Figure 2.2 shows the same illustration after it was "touched up" by hand to correct for overlap.

Note that one bond distance label was drawn in perspective along the bond, and the other was drawn as a regular label parallel to the page.

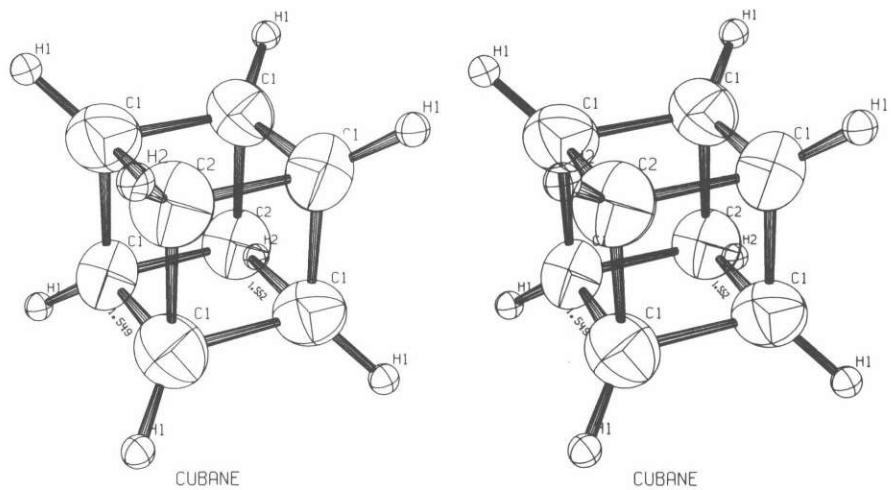


Fig. 2.1. The Sample Figure Cubane Before Retouching.

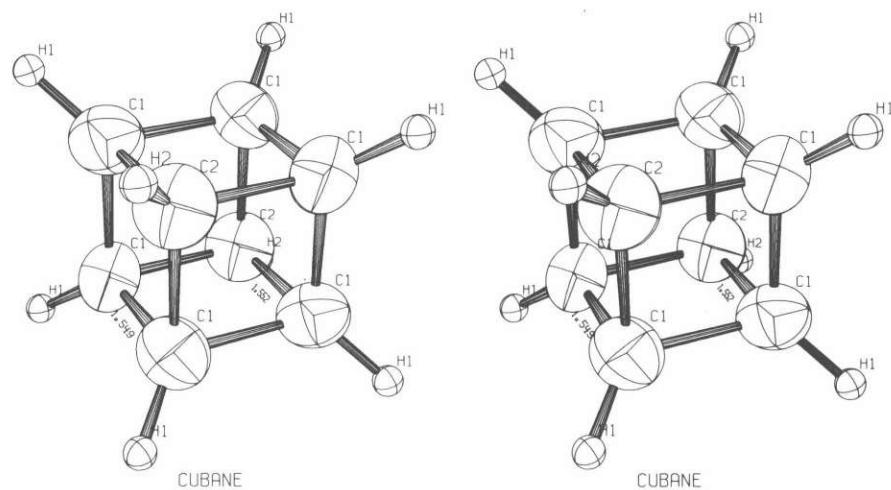


Fig. 2.2. The Sample Figure Cubane After Retouching.

2.4.5 Listing of Sample Input and Output. — 2.4.5.1 Listing of Input Cards. —

CUBANE (E.B.FLEISCHER (1964) J.A.C.S. 86,3889)
 5.34 5.34 5.34 72.26 72.26 72.26 EXAM0010
 0 1 0 0 0 0 0 0 0 0 0 0 EXAM0020
 0 0 0 1 0 0 0 0 0 0 0 0 EXAM0030
 0 0 1 0 0 0 0 0 0 0 0 0 EXAM0040
 0 -1 0 0 0 0 -1 0 0 0 0 0 EXAM0050
 0 0 0 -1 0 0 -1 0 0 0 0 -1 EXAM0060
 0 0 -1 0 0 0 0 0 0 0 0 0 EXAM0070
 0 0 -1 0 0 0 0 0 -1 0 0 0 EXAM0080
 CI -.18711 .19519 .10706 0 EXAM0090
 .04100 .04250 .04500 -.00420 -.01420 -.00510 0 EXAM0100
 C2 .11546 .11546 .11546 0 EXAM0110
 .04680 .04680 .04680 -.01430 -.01430 -.01430 0 EXAM0120
 HI -.32460 .34680 .18480 0 EXAM0130
 .10 7 EXAM0140
 H2 .21000 .21000 .21000 0 EXAM0150
 .10 7 EXAM0160
 ORGN 0 0 0 0 0 EXAM0170
 3 101 155501 2 1 4 3.61 EXAM0180
***** FIND ALL NEIGHBOR ATOMS AROUND CI AND C2 OUT TO 3.61 A ***** EXAM0200
 3 102 155501 2 1 4 1.8 EXAM0210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS ***** EXAM0220
 3 201 EXAM0230
***** INITIALIZE CALCOMP PLOT PACKAGE ***** EXAM0240
 3 301 11. 11. 24. 1. EXAM0250
***** IXIXI BOUNDARY, 9X9 INSIDE 1 INCH MARGIN, VIEW FROM 24 INCHES **** EXAM0260
 3 303 0 EXAM0270
***** ELIMINATE ALL RETRACING ***** EXAM0280
 3 402 555501 5 1 4 3.2 EXAM0290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5 ***** EXAM0300
 3 501 555501 255501 155501 255501 155502 EXAM0310
***** ORGN AT DUMMY ATOM 5, VECTORS ALONG 2 EDGES OF CUBANE ***** EXAM0320
 3 502 2 25. 1 28. EXAM0330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT X ***** EXAM0340
 3 503 2 3.0 EXAM0350
***** STEREO ROTATION OF 3.0 DEGREES ABOUT Y FOR LEFT EYE ***** EXAM0360
 3 604 0 0 0 1.54 EXAM0370
***** AUTO SCALE AND POSITION TO 9X9. 50 PERCENT PROBABILITY ELLIPSOIDS EXAM0380
 3 611 0 0 .9 0 EXAM0390
***** SHRINK SCALE BY 10 PERCENT FOR SAFETY ***** EXAM0400
 3 1101 EXAM0410
***** START SAVE SEQUENCE ***** EXAM0420
 3 412 555501 5 3 4 3.2 EXAM0430
***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION ***** EXAM0440
 3 715 4 0 1 0 .20 .60 .70 EXAM0450
***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. ***** EXAM0460
 3 410 EXAM0470
***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECEMEAL ***** EXAM0480
 3 401 355501 -455536 EXAM0490
***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN ***** EXAM0500
 3 712 .2 .35 .40 EXAM0510
***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH ***** EXAM0520
 3 402 555501 5 1 4 3.2 EXAM0530
***** ENCLOSER SPHERE WITH COMPLETE MODEL ***** EXAM0540
 2 812 EXAM0550
 3 1 4 1 4 4 .9 1.6 .04 EXAM0560
***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG ***** EXAM0570
 3 906 155504 155503 0 0 .15 0 -.4 EXAM0580
***** LABEL UNIQUE C-C BCNDS . CAPTION # CUBANE ***** EXAM0590
 916 255504 155505 0 0 .15 0 -.4 EXAM0600
 3 902 555501 0 0 1.0 .25 0 0 EXAM0610
 CUBANE EXAM0620
 3 1102 EXAM0630
***** END OF SAVE SEQUENCE ***** EXAM0640
 3 202 9. EXAM0650

***** ADVANCE PLOTTER 9 INCHES ALONG X FOR RIGHT EYE VIEW *****	EXAM0660
3 503 2 -3.0	EXAM0670
***** STEREO ROTATION FOR RIGHT EYE *****	EXAM0680
3 1103	EXAM0690
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE VIEW *****	EXAM0700
3 202 20.	EXAM0710
***** ADVANCE PLOTTER 20 INCHES *****	EXAM0720
3 202 0	EXAM0730
***** ADDS DUMMY PLOT TO MAGNETIC TAPE *****	EXAM0740
-1	EXAM0750

2.4.5.2 Listing of Output from the Monitor Output Tape of the Computer. —

CUBANE (E.B.FLEISCHER (1964) J.A.C.S. 86,3889)

DIRECT CELL PARAMETERS

A	B	C	ALPHA	BETA	GAMMA
5.340000	5.340000	5.340000	72.260 COSINE	72.260 0.30469811	72.260 0.30469811

RECIPROCAL CELL PARAMETERS

A*	B*	C*	ALPHA*	BETA*	GAMMA*
0.202207	0.202207	0.202207	103.506 COSINE	103.506 -0.23353916	103.506 -0.23353916

SYMMETRY TRANSFORMATIONS

NO.	TRANSFORMED X	TRANSFORMED Y	TRANSFORMED Z
1	1. X 0. Y 0. Z	0. X 1. Y 0. Z	0. X 0. Y 1. Z
2	0. X 0. Y 1. Z	1. X 0. Y 0. Z	0. X 1. Y 0. Z
3	0. X 1. Y 0. Z	0. X 0. Y 1. Z	1. X 0. Y 0. Z
4	0. X 0. Y 0. Z	0. X -1. Y 0. Z	0. X 0. Y -1. Z
5	0. X 0. Y -1. Z	-1. X 0. Y 0. Z	0. X -1. Y 0. Z
6	0. X -1. Y 0. Z	0. X 0. Y -1. Z	-1. X 0. Y 0. Z

NO. ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23	TYPE
1 CI	-0.187110	0.195190	0.107060	0.041000	0.042500	0.045000	-0.004200	-0.014200	-0.005100	0.
2 C2	0.115460	0.115460	0.115460	0.046800	0.046800	0.046800	-0.014300	-0.014300	-0.014300	0.
3 HI	-0.324600	0.346800	0.184800	0.100000	-0.	-0.	-0.	-0.	-0.	7.
4 H2	0.210000	0.210000	0.210000	0.100000	-0.	-0.	-0.	-0.	-0.	7.
5 ORGN	0.	0.	0.	-0.	-0.	-0.	-0.	-0.	-0.	0.

NO. ATOM	X	Y	Z	RMSD 1	RMSD 2	RMSD 3
1 CI	-0.187110	0.195190	0.107060	0.204899	0.239856	0.255794
2 C2	0.115460	0.115460	0.115460	0.205704	0.247733	0.247733
3 HI	-0.324600	0.346800	0.184800	0.100000	0.100000	0.100000
4 H2	0.210000	0.210000	0.210000	0.100000	0.100000	0.100000
5 ORGN	0.	0.	0.	0.100000	0.100000	0.100000

CUBANE (E.B.FLEISCHER (1964) J.A.C.S. 86,3889)

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES

X VECTOR	Y VECTOR	Z VECTOR
0.1872659E-00	-0.5990827E-01	-0.4722319E-01
0.	0.1966152E-00	-0.4722319E-01
0.	0.	0.2022067E-00

POST-FACTOR TRANSFORMATION MATRIX

0.5340000E 01	0.4470348E-07	0.2980232E-07
0.1627088E 01	0.5086078E 01	0.2980232E-07
0.1627088E 01	0.1187798E 01	0.4945434E 01

((((INSTRUCTION 101))))

0.1555010E 06 0.2000000E 01 0.1000000E 01 0.4000000E 01 0.3610000E 01 -0. -0.

***** FIND ALL NEIGHBOR ATOMS AROUND CI AND C2 OUT TO 3.61 A *****

FROM ATOMS	TO ATOMS	WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
CODE (MIN MAX)	(MIN MAX)	A B C

101 155501 2 1 4

3.610 -0. -0.

VECTORS FROM ATOM (1,55501) TO ATOMS I THROUGH 4

CI	HI	(1,55501)-0.1871 0.1952 0.1071	(3,55501)-0.3246 0.3468 0.1848	D # 1.012
CI	CI		(1,55505)-0.1071 0.1871-0.1952	D # 1.549
CI	CI		(1,55506)-0.1952-0.1071 0.1871	D # 1.549
CI	C2		(2,55501) 0.1155 0.1155 0.1155	D # 1.552
CI	CI		(1,55502) 0.1071-0.1871 0.1952	D # 2.183
CI	CI		(1,55503) 0.1952 0.1071-0.1871	D # 2.183
CI	C2		(2,55504)-0.1155-0.1155-0.1155	D # 2.202
CI	HI		(3,55506)-0.3468-0.1848 0.3246	D # 2.282
CI	HI		(3,55505)-0.1848 0.3246-0.3468	D # 2.306
CI	H2		(4,55501) 0.2100 0.2100 0.2100	D # 2.376
CI	CI		(1,55504) 0.1871-0.1952-0.1071	D # 2.677
CI	HI		(3,55502) 0.1848-0.3246 0.3468	D # 3.052
CI	HI		(3,55503) 0.3468 0.1848-0.3246	D # 3.069
CI	H2		(4,45501)-0.7900 0.2100 0.2100	D # 3.077
CI	H2		(4,56504)-0.2100 0.7900-0.2100	D # 3.096
CI	H2		(4,55504)-0.2100-0.2100-0.2100	D # 3.175
CI	HI		(3,55605)-0.1848 0.3246 0.6532	D # 3.200
CI	HI		(3,45603)-0.6532 0.1848 0.6754	D # 3.284
CI	HI		(3,46504)-0.6754 0.6532-0.1848	D # 3.388
CI	C2		(2,56504)-0.1155 0.8845-0.1155	D # 3.609

VECTORS FROM ATOM (2,55501) TO ATOMS I THROUGH 4

C2	H2	(2,55501) 0.1155 0.1155 0.1155	(4,55501) 0.2100 0.2100 0.2100	D # 1.109
C2	CI		(1,55501)-0.1871 0.1952 0.1071	D # 1.552
C2	CI		(1,55502) 0.1071-0.1871 0.1952	D # 1.552
C2	CI		(1,55503) 0.1952 0.1071-0.1871	D # 1.552
C2	CI		(1,55504) 0.1871-0.1952-0.1071	D # 2.202
C2	CI		(1,55505)-0.1071 0.1871-0.1952	D # 2.202
C2	CI		(1,55506)-0.1952-0.1071 0.1871	D # 2.202
C2	HI		(3,55501)-0.3246 0.3468 0.1848	D # 2.273
C2	HI		(3,55502) 0.1848-0.3246 0.3468	D # 2.273
C2	HI		(3,55503) 0.3468 0.1848-0.3246	D # 2.273
C2	C2		(2,55504)-0.1155-0.1155-0.1155	D # 2.710
C2	HI		(3,55504) 0.3246-0.3468-0.1848	D # 3.091
C2	HI		(3,55505)-0.1848 0.3246-0.3468	D # 3.091
C2	HI		(3,55506)-0.3468-0.1848 0.3246	D # 3.091
C2	HI		(3,56504) 0.3246 0.6532-0.1848	D # 3.181
C2	HI		(3,55605)-0.1848 0.3246 0.6532	D # 3.181
C2	HI		(3,65506) 0.6532-0.1848 0.3246	D # 3.181
C2	CI		(1,56504) 0.1871 0.8048-0.1071	D # 3.609
C2	CI		(1,55605)-0.1071 0.1871 0.8048	D # 3.609
C2	CI		(1,65506) 0.8048-0.1071 0.1871	D # 3.609

|||| INSTRUCTION 102))))
0.155501E 06 0.2000000E 01 0.1000000E 01 0.4000000E 01 0.1800000E 01 -0. -0.

***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****

FROM ATOMS TO ATOMS WITH RADIUS OR, IF A BOX, WITH SEMIDIIMENSIONS
CODE (MIN MAX) (MIN MAX) A B C

102 155501 2 1 4 1.800 -0. -0.

VECTORS FROM ATOM (1,55501) TO ATOMS 1 THROUGH 4
C1 H1 (1,55501)-0.1871 0.1952 0.1071 (3,55501)-0.3246 0.3468 0.1848 D # 1.012
C1 C1 (1,55501)-0.1071 0.1871-0.1952 D # 1.549
C1 C1 (1,55501)-0.1952-0.1071 0.1871 D # 1.549
C1 C2 (2,55501) 0.1155 0.1155 0.1155 D # 1.552

ANGLES AROUND ATOM 1
H1 C1 C1 (3,55501) (1,55501) (1,55501) 124.69
H1 C1 C1 (3,55501) (1,55501) (1,55506) 127.16
H1 C1 C2 (3,55501) (1,55501) (2,55501) 123.52
C1 C1 C1 (1,55505) (1,55501) (1,55506) 89.60
C1 C1 C2 (1,55505) (1,55501) (2,55501) 90.48
C1 C1 C2 (1,55506) (1,55501) (2,55501) 90.48

VECTORS FROM ATOM (2,55501) TO ATOMS 1 THROUGH 4
C2 H2 (2,55501) 0.1155 0.1155 0.1155 (4,55501) 0.2100 0.2100 0.2100 D # 1.109
C2 C1 (2,55501)-0.1871 0.1952 0.1071 D # 1.552
C2 C1 (1,55502) 0.1071-0.1871 0.1952 D # 1.552
C2 C1 (1,55503) 0.1952 0.1071-0.1871 D # 1.552

ANGLES AROUND ATOM 2
H2 C2 C1 (4,55501) (2,55501) (1,55501) 125.66
H2 C2 C1 (4,55501) (2,55501) (1,55502) 125.66
H2 C2 C1 (4,55501) (2,55501) (1,55503) 125.66
C1 C2 C1 (1,55501) (2,55501) (1,55502) 89.44
C1 C2 C1 (1,55501) (2,55501) (1,55503) 89.44
C1 C2 C1 (1,55502) (2,55501) (1,55503) 89.44

((((INSTRUCTION 201))))
-0. -0. -0. -0. -0. -0. -0.

***** INITIALIZE CALCOMP PLOT PACKAGE *****

((((INSTRUCTION 301))))
0.1100000E 02 0.1100000E 02 0.2400000E 02 0.1000000E 01 -0. -0. -0.

***** IIXII BOUNDARY, 9X9 INSIDE 1 INCH MARGIN, VIEW FROM 24 INCHES *****

PLOT LIMITS 11.00 BY 11.00 IN. INCLUDING 1.00 IN. MARGIN
VIEW DISTANCE 24.000 INCHES

((((INSTRUCTION 303))))
0. -0. -0. -0. -0. -0. -0.

***** ELIMINATE ALL RETRACING *****

RETRACE DISPLACEMENT # 0. INCH

((((INSTRUCTION 402))))
 0.5555010E 06 0.5000000E 01 0.1000000E 01 0.4000000E 01 0.3200000E 01 -0. -0.

***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5 *****

FROM ATOMS TO ATOMS WITH RADIUS OR, IF A BOX, WITH SEMI DIMENSIONS
 CODE (MIN MAX) (MIN MAX) A B C

402	555501	5	1	4	3.200	-0.	-0.
-----	--------	---	---	---	-------	-----	-----

VECTORS FROM ATOM (5,55501) TO ATOMS 1 THROUGH 4

CONTENTS OF ATOMS ARRAY

155501.	255501.	355501.	455501.	155502.	355502.	155503.	355503.	155504.	255504.
355504.	455504.	155505.	355505.	155506.	355506.				

((((INSTRUCTION 501))))
 0.5555010E 06 0.2555010E 06 0.1555010E 06 0.2555010E 06 0.1555020E 06 -0. 0.

***** ORGN AT DUMMY ATOM 5, VECTORS ALONG 2 EDGES OF CUBANE *****

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES POST-FACTOR TRANSFORMATION MATRIX

X VECTOR	Y VECTOR	Z VECTOR			
-0.1950172E-00	-0.5332417E-01	0.3517815E-02	-0.5161574E 01	0.2128974E-00	0.1352193E 01
0.5138884E-01	0.4031208E-02	0.1955262E-00	-0.2760937E-00	0.1350080E 01	0.5159133E 01
-0.5414101E-02	0.1954783E-00	-0.5144393E-01	-0.1402323E 01	0.5145891E 01	0.2624691E-00

((((INSTRUCTION 502))))
 0.2000000E 01 0.2500000E 02 0.1000000E 01 0.2800000E 02 -0. -0. -0.

***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT X *****

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES POST-FACTOR TRANSFORMATION MATRIX

X VECTOR	Y VECTOR	Z VECTOR			
-0.1752589E-00	-0.8727205E-01	0.5055148E-01	-0.4106513E 01	-0.1411455E 01	0.3108044E 01
0.1292070E-00	-0.6943834E-01	0.1391812E-00	0.1930118E 01	-0.1057867E 01	0.4865301E 01
-0.2664798E-01	0.1934115E-00	0.5262520E-01	-0.1160012E 01	0.4153645E 01	0.3149160E 01

((((INSTRUCTION 503))))
 0.2000000E 01 0.3000000E 01 -0. -0. -0. -0.

***** STEREO ROTATION OF 3.0 DEGREES ABOUT Y FOR LEFT EYE *****

ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES POST-FACTOR TRANSFORMATION MATRIX

X VECTOR	Y VECTOR	Z VECTOR			
-0.1723731E-00	-0.8727205E-01	0.5965454E-01	-0.3938223E 01	-0.1411455E 01	0.3318703E 01
0.1363141E-00	-0.6943834E-01	0.1322283E-00	0.2182103E 01	-0.1057867E 01	0.4757619E 01
-0.2385727E-01	0.1934115E-00	0.5394772E-01	-0.9936078E 00	0.4153645E 01	0.3205554E 01

((((INSTRUCTION 604))))
 0. 0. 0. 0.1540000E 01 -0. -0. -0.

***** AUTO SCALE AND POSITION TO 9X9. 50 PERCENT PROBABILITY ELLIPSOIDS

ORIGIN POINT IN PLOTTER COORD.(5.26 , 5.89) IN.
OVERALL SCALE # 2.196 INCH/ANGSTROM ELLIPSOID SCALE # 1.540
VIEW DISTANCE 24.000 INCHES

((((INSTRUCTION 611))))
0. 0. 0.9000000E 00 0. -0. -0. -0.

***** SHRINK SCALE BY 10 PERCENT FOR SAFETY *****

ORIGIN POINT IN PLOTTER COORD.(5.26 , 5.89) IN.
OVERALL SCALE # 1.977 INCH/ANGSTROM ELLIPSOID SCALE # 1.540
VIEW DISTANCE 24.000 INCHES

((((INSTRUCTION 1101))))
-0. -0. -0. -0. -0. -0. -0.

***** START SAVE SEQUENCE *****

((((INSTRUCTION 412))))
0.5555010E 06 0.5000000E 01 0.3000000E 01 0.4000000E 01 0.3200000E 01 -0. -0.

***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION *****

FROM ATOMS CODE (MIN MAX)	TO ATOMS (MIN MAX)	WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS	A	B	C
412 555501	5 3 4	3.200	-0.	-0.	

23

VECTORS FROM ATOM (5,555501) TO ATOMS 3 THROUGH 4

CONTENTS OF ATOMS ARRAY
155501. 255501. 155502. 155503. 155504. 255504. 155505. 155506.

((((INSTRUCTION 715))))
0.4000000E 01 0. 0.1000000E 01 0. 0.2000000E-00 0.6000000E 00 0.7000000E 00

***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. *****

((((INSTRUCTION 410))))
-0. -0. -0. -0. -0. -0. -0.

***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECemeAL *****

((((INSTRUCTION 401))))
0.3555010E 06 -0.4555060E 06 -0. -0. -0. -0. -0.

***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN *****

CONTENTS OF ATOMS ARRAY
355501. 455501. 355502. 355503. 355504. 455504. 355505. 355506.

((((INSTRUCTION 712))))
-0. -0. -0. 0.2000000E-00 0.3500000E-00 0.4000000E-00

***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH *****

((((INSTRUCTION 402))))
0.5555010E 06 0.5000000E 01 0.1000000E 01 0.4000000E 01 0.3200000E 01 -0. -0.

***** ENCLOSER SPHERE WITH COMPLETE MODEL *****

FROM ATOMS TO ATOMS WITH RADIUS OR, IF A BOX, WITH SEMIDIIMENSIONS
CODE (MIN MAX) (MIN MAX) A B C
402 555501 5 1 4 3.200 -0. -0.

VECTORS FROM ATOM (5,555501) TO ATOMS I THROUGH 4

CONTENTS OF ATOMS ARRAY
355501. 455501. 355502. 355503. 355504. 455504. 355505. 355506. 155501. 255501.
155502. 155503. 155504. 255504. 155505. 155506.

((((INSTRUCTION 812))))
-0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0.

***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG *****

BOND SELECTION CODES

(SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)(BOND)(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
(MIN MAX)(MIN MAX)(TYPE) (MIN MAX)(RADIUS)(HEIGHT OFFSET)(HEIGHT OFFSET)(NUMBER)
I 4 I 4 4 0.90 1.60 0.0400 -0. -0. -0. -0. -0.

FAULT NG # 14 455504. 800

24

((((INSTRUCTION 906))))
0.1555040E 06 0.1555030E 06 0. 0. 0.1500000E-00 0. -0.4000000E-00

***** LABEL UNIQUE C-C BONDS . CAPTION # CUBANE *****

((((INSTRUCTION 916))))
0.2555040E 06 0.1555050E 06 0. 0. 0.1500000E-00 0. -0.4000000E-00

((((INSTRUCTION 902))))
0.5555010E 06 0. 0. 0.1000000E 01 0.2500000E-00 0. 0.

CUBANE

((((INSTRUCTION 1102))))
-0. -0. -0. -0. -0. -0. -0.

***** END OF SAVE SEQUENCE *****

((((INSTRUCTION 202))))
 0.9000000E 01 -0. -0. -0. -0. -0.

***** ADVANCE PLOTTER 9 INCHES ALONG X FOR RIGHT EYE VIEW *****

((((INSTRUCTION 503))))
 0.2000000E 01 -0.3000000E 01 -0. -0. -0. -0.

***** STEREO ROTATION FOR RIGHT EYE *****

ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES	POST-FACTOR TRANSFORMATION MATRIX		
X VECTOR	Y VECTOR	Z VECTOR	
-0.1776644E-00	-0.8727205E-01	0.4130986E-01	-0.4263548E 01 -0.1411455E 01 0.2888866E 01
0.1217458E-00	-0.6943834E-01	0.1457526E-00	0.1672843E 01 -0.1057867E 01 0.4959648E 01
-0.2936565E-01	0.1934115E-00	0.5115843E-01	-0.1323236E 01 0.4153645E 01 0.3084133E 01

((((INSTRUCTION 1103))))
 -0. -0. -0. -0. -0. -0. -0.

***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE VIEW *****

((((INSTRUCTION 412))))
 0.5555010E 06 0.5000000E 01 0.3000000E 01 0.4000000E 01 0.3200000E 01 -0. -0.

***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION *****

FROM ATOMS	TO ATOMS	WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS	
CODE (MIN MAX)	(MIN MAX)	A B C	
412 555500	4 3 4	3.200	-0. -0.

VECTORS FROM ATOM (5,55500) TO ATOMS 3 THROUGH 4

CONTENTS OF ATOMS ARRAY
 155501. 255501. 155502. 155503. 155504. 255504. 155505. 155506.

((((INSTRUCTION 715))))
 0.4000000E 01 0. 0.9999999E 00 0. 0.2000000E-00 0.6000000E 00 0.7000000E 00

***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. *****

((((INSTRUCTION 410))))
 -0. -0. -0. -0. -0. -0. -0.

***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECEMEAL *****

((((INSTRUCTION 401))))
 0.3555010E 06 -0.4555060E 06 -0. -0. -0. -0. -0.

***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN *****

CONTENTS OF ATOMS ARRAY
 355501. 455501. 355502. 355503. 355504. 455504. 355505. 355506.
 ((((INSTRUCTION 712))))
 -0. -0. -0. -0. 0.2000000E-00 0.3500000E-00 0.4000000E-00
 ***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH *****
 ((((INSTRUCTION 402))))
 0.555501E 06 0.5000000E 01 0.9999999E 00 0.4000000E 01 0.3200000E 01 -0. -0.
 ***** ENCLOSER SPHERE WITH COMPLETE MODEL *****
 FROM ATOMS TO ATOMS WITH RADIUS OR, IF A BOX, WITH SEMIDIIMENSIONS
 CODE (MIN MAX) (MIN MAX) A B C
 402 555500 4 1 4 3.200 -0. -0.
 VECTORS FROM ATOM (5,55500) TO ATOMS I THROUGH 4
 CONTENTS OF ATOMS ARRAY
 355501. 455501. 355502. 355503. 355504. 455504. 355505. 355506. 155501. 255501.
 155502. 155503. 155504. 255504. 155505. 155506.
 ((((INSTRUCTION 812))))
 -0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0. -0.
 ***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG *****
 BOND SELECTION CODES
 (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)(BOND)(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
 (MIN MAX)(MIN MAX) (TYPE) (MIN MAX)(RADIUS)(HEIGHT OFFSET)(HEIGHT OFFSET)(NUMBER)
 1 4 1 4 4 0.90 1.60 0.0400 -0. -0. -0. -0. -0. -0.
 FAULT NG # 14 455504. 800
 ((((INSTRUCTION 906))))
 0.1555040E 06 0.1555030E 06 0. 0. 0.1500000E-00 0. -0.4000000E-00
 ***** LABEL UNIQUE C-C BONDS . CAPTION # CUBANE *****
 ((((INSTRUCTION 916))))
 0.2555040E 06 0.1555050E 06 0. 0. 0.1500000E-00 0. -0.4000000E-00
 ((((INSTRUCTION 902))))
 0.555501E 06 0. 0. 0.9999999E 00 0.2500000E-00 0. 0.
 CUBANE

((((INSTRUCTION 1102))))
-0. -0. -0. -0. -0. -0. -0.
***** END OF SAVE SEQUENCE *****
((((INSTRUCTION 202))))
0.200000E 02 -0. -0. -0. -0. -0.
***** ADVANCE PLOTTER 20 INCHES *****
((((INSTRUCTION 202))))
0. -0. -0. -0. -0. -0. -0.
***** ADDS DUMMY PLOT TO MAGNETIC TAPE *****
((((INSTRUCTION -1))))

3. DETAILED OPERATING INSTRUCTIONS

3.1 Definitions

Several conventions must be defined before the instructions can be explained.

3.1.1 Atom Designator Code (ADC) and Addressable Point. — In order to specify a particular atom in the crystal within a reasonable distance from the crystallographically defined origin, the following five-component atom designator code word (ADC) is used.

$$\text{ADC} = \text{AN} * 10^5 + (\text{TA} + 5) * 10^4 + (\text{TB} + 5) * 10^3 + (\text{TC} + 5) * 10^2 + \text{SN}$$

where

$\text{AN} = \text{ATOM NUMBER}$ ($0 \leq \text{AN} \leq \text{NATOM} \leq 200$) = the sequential number of the atom in the input list of atoms in the asymmetric unit, which contains NATOM atoms. Atom zero is not in the input atom list but refers to the crystal origin point (0., 0., 0.).

$\text{TA}, \text{TB}, \text{TC} = \text{crystal lattice translation digits along cell edges } \mathbf{a}, \mathbf{b}, \text{ and } \mathbf{c}$. Each digit in ADC can range from 1 to 9; consequently, it is possible to move up to ± 4 lattice translations in any direction from the origin cell 5,5,5. In certain cases 0,0,0 is permitted in place of 5,5,5; however, a mixed translation designation such as 0,5,5 is not permitted.

$\text{SN} = \text{symmetry operator number}$ ($0 \leq \text{SN} \leq \text{NSYM} \leq 48$) = the numerical position of the symmetry operator in the input symmetry operator list which contains NSYM entries. Symmetry operator number zero is not in the input list but refers to an identity operator. However, the identity operation (corresponding to position x, y, z) must in general also be somewhere in the input symmetry operator list.

Example: An atom designation code of 3 47502 refers to atom 3 moved through symmetry operation 2, then translated -1 cell translation along \mathbf{a} , +2 cell translations along \mathbf{b} , and 0 cell translations along \mathbf{c} .

An *addressable point* in the crystal is any point for which an atom designator code exists. In general, the addressable region is approximately a $9 \times 9 \times 9$ block of unit cells.

3.1.2 Vector Designator Code (VDC). — A vector direction is specified by two atom designator codes. The vector direction is from the first to the second.

Example: 253704 263704 is a vector along the positive \mathbf{a} direction of the crystal lattice.

3.1.3 Atom Designator Run (ADR). — A straight run sequence of atoms can be defined using two atom designator codes with a negative sign preceding the second of the two. The run hierarchy is: first, atom number AN; second, symmetry operation SN; third, \mathbf{a} translation TA; fourth, \mathbf{b} translation TB; and last, \mathbf{c} translation TC.

Example: ADR (145502 - 245603) will generate the 8-atom run 145502, 245502, 145503, 245503, 145602, 245602, 145603, 245603.

3.1.4 Atom Number Run (ANR). — The Atom Number Run is a subset of the Atom Designator Run. In this case, only the atom number AN is allowed to change. Normally, an ANR is entered by using only the atom number (AN) values for the first and last members of the sequence without a minus sign.

Example: (1 4) will designate atoms 1, 2, 3, and 4 of the input list.

3.1.5 Vector Search Code (VSC). – A vector search code consists of two atom number runs and a distance range. It is used for finding interatomic distances which have a particular chemical significance, such as covalent and coordination bonds.

Example: Suppose that metal atoms are numbers 1 and 2 in the atom list and oxygen atoms are 6–12 and that the interatomic distance range between metals and oxygens is 1.9 Å to 2.4 Å. The metal-to-oxygen vectors can be specified by the vector search code (1 2) (6 12) (1.9 2.4). Several variations of this basic code are used in the program.

3.1.6 Sphere of Enclosure. – The sphere of enclosure specifies some or all of the atoms lying within a sphere of radius D_{max} about a given “origin” atom without the necessity of delineating each atom individually. This “sphere of enclosure” is said to contain a *complete population* if all addressable atoms within the D_{max} radius are included. If the sphere of enclosure contains only certain types of atoms which are derived from a group of sequential atoms in the input list, then the sphere is said to have a *partial population*. Finally, the population (complete or partial) of the sphere of enclosure can be screened as selectively as desired through the use of vector search codes (3.1.5), and the resulting content is called a *vector screened population*.

A sphere of enclosure can be centered on any addressable atom, but one should not use points in the outermost cells as centers because of the possibility of having nonaddressable points within the D_{max} radius.

3.1.7 Box of Enclosure. – This is a rectangular parallelepiped which can be centered about any addressable point and assigned arbitrary orientation and dimensions. This “box of enclosure” can have a *complete population* or a *partial population* as described for the sphere of enclosure (3.1.6). However, vector screening is not allowed with the box of enclosure.

3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems. – Many of the OR TEP calculations use fractional coordinates based on the crystal axes **a**, **b**, and **c** (triclinic coordinate system); but other steps necessitate the introduction of orthonormal base vector triplets (Cartesian coordinate systems). Two Cartesian systems (reference and working) are utilized. The reference (major) system is used for all operations except plotting, where the working (minor) system is used. For a right-eye or left-eye stereo view, the working system is moved from the reference system by rotation about an axis of the reference system. However, certain decisions made while plotting must still be referred to the reference system to maintain accurate stereopsis. The user can define and orient the two Cartesian systems through the instructions of series 500. Until a 500-series instruction is given, a “standard Cartesian system” is utilized for both the reference and working systems. The orthonormal base vectors of the standard system are oriented as follows:

$$\begin{aligned} \text{x axis along } & \mathbf{a}, \\ \text{y axis along } & (\mathbf{a} \times \mathbf{b}) \times \mathbf{a}, \\ \text{z axis along } & \mathbf{a} \times \mathbf{b} = \mathbf{c}^*, \end{aligned}$$

where **a**, **b**, and **c** are crystal axes and \times denotes the outer vector product (cross product). The symbol \mathbf{c}^* refers to a reciprocal axis.

3.1.9 Prime Parameters and Primer Constants. — In the process of mathematically describing an illustration to be machine drawn, many parameters must be used. The more basic among these parameters are called *Prime Parameters*. The values assigned to these prime parameters are often similar or identical from one problem to the next. The first thing OR TEP does is to call subroutine PRIME, which sets as many prime parameters as possible to reasonable, "in the ball park," *Primer Constants*. For example, the maximum plot dimensions (instruction 300 series) are set at 30.0 in. for x maximum and 11.0 in. for y maximum, and the overall scale for plotting (instruction 600 series) is set at 1.0 in./A. If the value assigned to a particular constant by the primer routine is satisfactory, the user does not have to reset this constant with OR TEP instructions.

3.2 Crystal Structure Data Input

3.2.1 Title Card. — FORMAT (12A6)

Columns

1–72 Title consisting of any desired alphanumeric identification information.
This will appear periodically in the output.

3.2.2 Cell Parameter Card. — FORMAT (6F9.6). Any one of the four following input alternatives may be used (no indicator is needed to specify which type).¹

Columns	Type A	Type B	Type C	Type D
1–9	a (A)	a (A)	a^* (A^{-1})	a^* (A^{-1})
10–18	b (A)	b (A)	b^* (A^{-1})	b^* (A^{-1})
19–27	c (A)	c (A)	c^* (A^{-1})	c^* (A^{-1})
28–36	α (deg)	$\cos \alpha$	α^* (deg)	$\cos \alpha^*$
37–45	β (deg)	$\cos \beta$	β^* (deg)	$\cos \beta^*$
46–54	γ (deg)	$\cos \gamma$	γ^* (deg)	$\cos \gamma^*$

The parameters a^* , etc., refer to the reciprocal unit cell such that $a \cdot a^* = 1$. All four types will be printed out regardless of which type was used for input.

3.2.3 Symmetry Cards ($1 \leq NSYM \leq 48$). — FORMAT (I1,F14.10, 3F3.0,2(F15.10,3F3.0)). The card will be interpreted in one of two ways, depending on the numerical value of the number in columns 70–72. If that number is < 5.0 , the card is interpreted as a crystallographic symmetry operation; but if the number is ≥ 5.0 , the card is interpreted as a general helix-screw symmetry operation² along the c^* crystal axis³

¹The routine assumes that $a \geq 1.0$ A, $a^* < 1.0 A^{-1}$, α (or α^*) $\geq 1.0^\circ$, and $|\cos \alpha|$ (or $|\cos \alpha^*|$) < 1.0 .

²The general helix-screw symmetry operation is not an allowed element of a crystallographic group, so that the molecular environment of the transformed unit will not in general be identical to that of the untransformed unit (unless the crystal is considered to be one dimensional). This input is simply an expedient for use in plotting helical polymer structure models with minimum input. In general it would be possible to produce the same results by specifying the complete crystallographic asymmetric unit and normal crystallographic symmetry transformations.

³This input mode is only meaningful if the cell angles α and β are 90° , so that c lies along c^* and the helix can continue uninterrupted from cell to cell along the c axis.

(third axis of the standard Cartesian system; see 3.1.8). The two symmetry types can be intermixed if desired.

Columns	(a) Crystallographic symmetry (70–72 \leq 5)	(b) Helix symmetry (70–72 \geq 5)
1	$\neq 0$ last card only	$\neq 0$ last card only
2–15	T_1	T_1
16–18	S_{11}	—
19–21	S_{12}	—
22–24	S_{13}	—
25–39	T_2	T_2
40–42	S_{21}	—
43–45	S_{22}	—
46–48	S_{23}	—
49–63	T_3	T_3
64–66	S_{31}	L
67–69	S_{32}	M
70–72	S_{33}	N

(a) Crystallographic symmetry: Transformed triclinic coordinates (X_1, Y_1, Z_1) are obtained from input triclinic coordinates (X, Y, Z) by

$$X_1 = T_1 + S_{11} X + S_{12} Y + S_{13} Z,$$

$$Y_1 = T_2 + S_{21} X + S_{22} Y + S_{23} Z,$$

$$Z_1 = T_3 + S_{31} X + S_{32} Y + S_{33} Z,$$

or in matrix notation

$$\mathbf{X}_1 = \mathbf{T} + \mathbf{S} \mathbf{X},$$

where

$$\mathbf{T} = (T_1, T_2, T_3) \text{ as fractions of cell edges.}$$

(b) Helix screw symmetry:

$$\mathbf{X}_1 = \mathbf{T} + \mathbf{S} \mathbf{X},$$

where

$$\mathbf{T} = (T_1, T_2, T_3 + L/N) \text{ as fractions of cell edge and}$$

\mathbf{S} = a counterclockwise rotation of $L \cdot M/N$ cycles about c^* axis.

For example, the Pauling and Corey right-handed alpha helix repeats after 5 turns and 18 residues and can be represented by 18 symmetry cards with $N = 18$; $M = 5$; $L = 0, 1, \dots, 17$; $T_1, T_2, T_3 = 0$. The input atom list contains the contents of one residue.

3.2.4 Atom Parameter Cards (1 \leq NATOM \leq 200). — Two cards are required for each input atom. The first contains the chemical symbol and positional parameters, and the second contains temperature factor

information or other information which specifies how the atom is to be represented on the drawing. The format allows the use of the atom parameter cards produced by the FORTRAN Least Squares Program OR FLS by Busing, Martin, and Levy (1962).⁴ Several alternate inputs are possible for each of the two cards, and the number in columns 55–63 denotes the type used on that particular card.

3.2.4.1 Positional Parameter Card. – FORMAT(A6,3X,5F9.6,F9.0)

Columns

1–6	Up to six alphanumeric characters centered in the six-place field			
7–9	Blank			
	Type 0	Type 1	Type 2	Type 3
10–18	—	—	—	x_0 (A) Cartesian
19–27	—	—	—	y_0 (A) Cartesian
28–36	x (fractional, crystal)	x (A, crystal)	x (A, Cartesian)	r (A) cylindrical
37–45	y (fractional, crystal)	y (A, crystal)	y (A, Cartesian)	ϕ ($^{\circ}$) cylindrical
46–54	z (fractional, crystal)	z (A, crystal)	z (A, Cartesian)	z (A) cylindrical
55–63	0 or blank	1	2	3

Type 0 is the normal input based on triclinic coordinates. Some authors give coordinates in A along the unit cell vector; type 1 would be used in such a case. Type 2 allows one to place a model described in Cartesian coordinates onto a general triclinic lattice. The orientation of the Cartesian system x y z in the general lattice a b c is the standard type described in 3.1.8 with x along a and z along c^* . Type 3 is similar to type 2 except that cylindrical coordinates r , ϕ , z are used and the axis of the system can be displaced from zero in the x y Cartesian plane by the displacement x_0 , y_0 . Cylindrical coordinates are often used in the literature to describe a helical structure. The x_0 , y_0 translation should be zero if helical symmetry operators are used. This translation feature is meant to be used in explicitly describing the contents of a multiple helix cell.

3.2.4.2 Temperature Factor Card. – FORMAT(I1,F8.6,5F9.6,F9.0)

Columns

1	A sentinel \neq 0 for last atom only			
	Type 0,1,2,3	Type 4,5	Type 6	Type 7
2–9	b_{11}	U_{11}	B	R
10–18	b_{22}	U_{22}	0	0
19–27	b_{33}	U_{33}	0	0
28–36	b_{12}	U_{12}	0	$\} [VDC_1]$
37–45	b_{13}	U_{13}	0	$\} [VDC_2]$
46–54	b_{23}	U_{23}	0	$\} [VDC_2]$
55–63	0,1,2,3	4,5	6 (or 0)	7
			6 (or 0)	7

⁴W. R. Busing and H. A. Levy, *A Fortran Crystallographic Least-Squares Program*, ORNL-TM-305 (Nov. 21, 1962).

The coefficients b_{ij} ($i,j = 1,2,3$) of the anisotropic temperature factor, types 0–3, are defined as follows:
The complete temperature factor is

$$(Base) \left\{ -(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + C b_{12}hk + C b_{13}hl + C b_{23}kl) \right\}$$

where in type 0: Base = e, C = 2;

type 1: Base = e, C = 1;

type 2: Base = 2, C = 2;

type 3: Base = 2, C = 1.

The coefficients U_{ij} ($i,j = 1,2,3$) of the anisotropic temperature factor, types 4 and 5, are defined as follows: The complete temperature factor is

$$\exp \left\{ -\frac{1}{4} (\mathbf{a}_1^{*2} U_{11} h^2 + \mathbf{a}_2^{*2} U_{22} k^2 + \mathbf{a}_3^{*2} U_{33} l^2 + C \mathbf{a}_1^{*} \mathbf{a}_2^{*} U_{12} hk + C \mathbf{a}_1^{*} \mathbf{a}_3^{*} U_{13} hl + C \mathbf{a}_2^{*} \mathbf{a}_3^{*} U_{23} kl) \right\},$$

where \mathbf{a}_1^* , \mathbf{a}_2^* , \mathbf{a}_3^* are reciprocal cell dimensions and in type 4, C = 2; in type 5, C = 1. Type 6 allows the input of the Debye-Waller isotropic temperature factor B , which is used as follows:

$$\exp(-B \sin^2 \theta/\lambda^2),$$

where λ is the wavelength and θ is the Bragg angle. The parameter B is related to mean-square displacement $\overline{\mu^2}$ of the atom from its mean position by the relation

$$B = 8\pi^2 \overline{\mu^2}.$$

When the isotropic temperature factor is used, the atom is represented as an isotropic ellipsoid (sphere) with equal principal axes of length μ . When the field in columns 19–27 is 0 or blank, the directions of the principal axes are along the standard Cartesian system axes (see 3.1.8). However, one can reorient these arbitrary orthogonal vectors by using the two vector designator codes VDC₁ and VDC₂; then the three new principal-axis vectors will be VDC₁, (VDC₁ × VDC₂), and VDC₁ × (VDC₁ × VDC₂). This is strictly an artistic feature of no physical significance.

Type 7 allows the input of arbitrary spheres of radius $\bar{\mu} = R$ in angstroms. The vector triplet orientation is specified as with type 6. An additional feature allows one to use a completely blank card (except perhaps column 1) for a temperature factor card. In this case the program assumes type 7 with an $R = 0.1$ Å.

3.3 Instruction Input

The instructions are the commands used in programming an illustration, and there is no required sequence for the instructions, except as indicated by the programming logic. Some instructions require trailer cards, which may have three different formats. The program is informed what the format of the next card will be with the “look ahead” field, columns 1 to 3. The program action is also influenced by this information.

"Look ahead" (columns 1-3)	Next card will be -	Program action
0 or blank	Format No. 0, a new instruction	Execute present instruction; then read next card.
1	Format No. 1, continuation of present instruction	Read continuation card; then check "Look ahead."
2	Format No. 2, vector search code	Read (VSC) card; then check "Look ahead."
3	Format No. 3, alphanumeric info.	Read alphanumeric info. and execute instruction; then read next card.

3.3.1 Instruction Cards. — 3.3.1.1 The Format No. 0 Instruction Card. — FORMAT(I3,I6,7F9.0)

Columns

1-3	"Look ahead" (0,1,2,3)
4-9	Instruction number
10-18	1st parameter
19-27	2nd parameter
.	.
.	.
.	.
64-72	7th parameter

3.3.1.2 Format No. 1, Instruction Continuation Card. — FORMAT(I3,I6,7F9.0) A maximum of 19 continuation cards per instruction is permitted.

Columns

1-3	"Look ahead" (0,1,2,3)
4-9	Blank
10-18	8th parameter, or 15th, . . . , or 134th
.	.
.	.
64-72	14th parameter, or 21st, . . . , or 140th

3.3.1.3 Format No. 2, Vector Search Code (VSC) Card. — FORMAT(I3,6X,5I3,8F6.0) A maximum of twenty VSC cards is allowed. These cards can be entered with any instruction, but only certain instructions will use them. They must be entered with the particular instructions that require them; that is, they are not held over. Table 3.1 will be referred to as the individual instructions are explained.

Table 3.1. Vector Search Code Cards

Columns	Search Instructions		Bond Plotting Instructions		
	101 402		801	802	803
	102 412				
1-3	Look ahead		Look ahead	Look ahead	Look ahead
4-9	-		-	-	-
10-12	} ORG. ANR		-	} ANR (A)	} ANR (A)
13-15			-		
16-18	} TAR. ANR		-	} ANR (B)	} ANR (B)
19-21			-		
22-24	-	Bond type	Bond type		-
25-30	D min (A)		-	D min (A)	D min (A)
31-36	D max (A)		-	D max (A)	D max (A)
37-42	-	Bond radius (A)	Bond radius (A)		-
43-48	-	Perspective label hgt. (in.)	Perspective label hgt. (in.)		-
49-54	-	Perpendicular displ. (in.)	Perpendicular displ. (in.)		-
55-60	-	Nonperspective label hgt. (in.)	Nonperspective label hgt. (in.)		-
61-66	-	Perpendicular displ. (in.)	Perpendicular displ. (in.)		-
67-72	-	Digits indicator	Digits indicator		-

3.3.1.4 Format No. 3, Labeling Card. — FORMAT(12A6)

Columns

1-72 Up to 72 digits of alphanumeric label information centered about columns 36 and 37.
 Note: There is no "look ahead" column in Format No. 3; the next card must be a new instruction card. Instructions 902, 903, and 913 are the only ones which require this input. It may be used with other instructions as a device to transfer comments about the particular instruction to the monitor output listing.

3.3.2 Structure Analysis Instructions (100 Series). — This series of instructions is not connected with drawing illustrations. It is used to obtain on the standard output medium of the computer a convenient tabulation of the chemically interesting aspects of a crystal structure, such as interatomic distances, interatomic angles, and principal axes of thermal motion.

3.3.2.1 Instructions 101 and 102. — These instructions call subroutine SEARCH, which finds all "target" atoms within a sphere of enclosure of radius D max about a particular "origin" atom. The instruction card has an atom number run (see 3.1.4) of origin atoms (Org. ANR) and an atom number run of target atoms (Tar. ANR). The Org. ANR allows one to calculate several spheres successively with a printout of results after each one. For example, suppose there are nine atoms in the input list

and we want the total surroundings of atoms 365502, 465502, and 565502 out to a maximum radius, D_{max} , of 4 Å. The Org. ANR is designated (365502, 5) or (365502, 565502)⁵ and the Tar. ANR is designated (1,9). Further selection of the interatomic vectors from a particular origin atom to the target atoms which fall within the limiting sphere is possible with vector search code (VSC) cards of Format No. 2 (see 3.3.1), which can be entered with the instruction. If VSC cards are present, then the vectors must also satisfy one of the VSC's in order to be saved. A VSC card to specify the selection of a shell of vectors in the above example might be coded as follows: Org. ANR (3,5) Tar. ANR (1,9) Dist. range (2.0, 2.7). More selective VSC's are also possible. They are meant to be based on known interatomic distance ranges, such as those tabulated in Vol. III of the *International Tables for X-Ray Crystallography*.⁶

Vectors found about a particular origin atom are stored in a table of dimension 200 sorted on distance. Duplicate vectors (not duplicate distances) are eliminated. If more than 200 acceptable atoms are found about an origin atom, the 200 shortest vectors are saved. At the end of the search about each origin atom, the distances are printed out along with the atom designator codes (ADC), chemical symbols, and triclinic crystal coordinates for the origin and target atoms. If the instruction is 102, all possible interatomic angles are also calculated and printed for the stored vectors. There will be $n(n - 1)/2$ angles for n vectors.

The tabulation of atom designator codes, which is obtained automatically when these instructions are given, is often useful for planning an illustration. Although the tabulation is complete within the addressable region of 9^3 cells, the computing time is generally only a matter of seconds per sphere unless a very large D_{max} is specified. Subroutine SEARCH is a rather elaborate routine designed to minimize computing time. This subroutine is also used for instructions 402 and 403, which are explained in 3.3.4.

Instruction card for instructions 101 and 102:

Columns

1–3	0 or 2 (look ahead)
4–9	101 or 102
10–18 } 19–27 }	ORIGIN (atom number run)
28–36 } 37–45 }	TARGET (atom number run)
46–54	D_{max} (Å)

3.3.2.2 *Instruction 103.* – Principal axes of thermal motion (or arbitrary spheres, according to the temperature factor input) for all atoms in the input list are calculated. The printout contains root-mean-

⁵For the origin sequence 355501, 455501, 555501, an Org. ANR input (3,5) is allowed as well as (355501,5) and (355501,555501); however, the Tar. ANR must always be designated as shown. In sect. 2.1, Org. ANR is designated as ORG 1, ORG 2; and Tar. ANR is denoted by TAR 1, TAR 2.

⁶H. Ondik and D. Smith, "Interatomic Distances in Inorganic Compounds," p. 257 in *International Tables for X-Ray Crystallography*, vol. III, ed. by K. Lonsdale, Kynoch, Birmingham, 1962.

square amplitudes of displacement along the principal axes of the trivariate normal probability density function and direction cosines for the principal axes relative to the reference Cartesian base vectors. A symmetric covariance dispersion matrix based on the reference Cartesian system is also printed out. The diagonal elements are the mean-square displacements along the reference Cartesian axes.

Columns

1-3	0 or blank (look ahead)
3-9	Blank
10-18	103

3.3.3 Plotter Control Instructions (200 Series). — The 200 series is a group of instructions that control the plotter initialization, frame advance, termination, and any other peripheral commands that are required for a particular equipment configuration or plotting package. When the program is modified for a different equipment configuration, these series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements. Instructions for controlling the CalComp 580 off-line magnetic tape plotting system⁷ are given here.

3.3.3.1 Instruction 201, Plot Package Initialization. — This instruction must be executed before any plotting can take place. It is a safe policy always to make this the first instruction card. It should be used only once per computer job regardless of how many plots are to be drawn during the job.

3.3.3.2 Instruction 202, Plot Terminate and Frame Advance. — This takes care of putting the correct plot termination information onto the magnetic tape to inform the plotter that the current plot is finished. It also allows advance of the paper so that the old plot is removed and new paper is in position for the next plot.

Columns	Instruction 201	Instruction 202
1-3	Blank	Blank
4-9	201	202
10-18	—	Plotter movement along x edge of paper in inches

3.3.4 Plot Boundary Instructions (300 Series). — This is a set of miscellaneous instructions for specifying the dimensions of the drawing, viewing distance, general lettering orientation, and pen displacement for line retracing.

3.3.4.1 Instruction 301. — This instruction defines the limiting x and y dimensions, in inches, of the plot boundary and the border indentations. The boundary dimensions must not exceed those allowed by the plotter. The program will prevent the pen from getting closer than 0.1 in. to any boundary. The border indentation is an equal margin inside the entire boundary. When automatic scaling is used (600

⁷The CalComp is an incremental plotter. The particular Benson-Lehner model available at Oak Ridge Central Data Processing Facility has also been used. The Benson-Lehner is an electromechanical x-y plotter with an analog converter. In general it seems that an incremental plotter is better suited to the requirement of OR TEP. The user should be warned that in the author's experience the magnetic tape plotting systems are notoriously troublesome; an annoying percentage of plot failures is to be expected because of equipment malfunctions.

series), the center points of the atoms are prevented from falling in the margin; but the atom representation, which has a finite size, may extend into that area. To compensate for the overlap, the border dimensions should be large when the overall drawing scale and the ellipsoid scale are expected to be large.

In addition, instruction 301 specifies the perspective viewing distance, in inches, from the plane of the drawing. An entry of 0 for view distance is used to indicate an infinite view distance, and the crystal structure is then mapped in parallel projection normal to the drawing board.

Columns		Primer Constant
1-3	—	—
4-9	301	—
10-18	Plot x limit (in inches)	30.
19-27	Plot y limit (in inches)	11.
28-36	View distance (in inches)	0. (parallel proj.)
37-45	Border (in inches)	0.5

3.3.4.2 Instruction 302, Title Rotation. — For regular titles and chemical symbols, the title rotation is specified with instruction 302. The lettering base line for all lettering is rotated counterclockwise by an angle theta, in degrees, from the x axis of the plotter. Although any value is allowed, 0° and -90° are the values most often used, so that, when one views the finished drawing, either the y plotter axis is vertical or the x plotter axis is vertical.

Columns		Primer Constant
1-3	Blank	—
4-9	302	—
10-18	Theta in degrees	0.

3.3.4.3 Instruction 303, Retrace Displacement. — For artistic purposes, certain lines are made heavier than others by retracing over the path several times with slight pen displacements (DISP) from the original path. For example, in drawing ellipsoids the forward half of the principal plane trace is made heavier than the hidden half so the eye does not confuse the two halves. In addition all regular lettering (but not perspective lettering) is gone over four times to give it boldface appearance. In preliminary runs or when the plotter is not of the incremental type, this embellishment may be objectionable to the user because of the increased computing and plotting times (particularly the latter). All retracing can be eliminated by setting DISP = 0. The primer parameter for DISP is 0.005 in., which is the resolution of the CalComp plotters at ORNL. For other plotters or for various inking pen sizes, DISP can be reset at the user's discretion.

Columns		Primer Constant
1-3	—	—
4-9	303	—
10-18	DISP (in inches)	0.005

3.3.5 Atom List Instructions (400 Series). — This series allows the user to specify which atoms are to be included in the illustration. The atom designators for the chosen atoms are stored in the ATOMS array for future use by other instructions. The ATOMS array can hold 500 atoms; but if the intended illustration has more than this, the illustration can be segmented and the segments drawn sequentially on the same plot. This technique may also be used when different parts of the drawing are to have different graphic representations. That is, we would define the first segment, draw it with the first representation, clear the ATOMS array, define the second segment, and draw it with the second graphic representation.

Groups of atoms are added to or eliminated from the ATOMS array (which is set to zero at the start of the program) with the 400 and 410 series respectively. The groups can be denoted by atom designator runs (see 3.1.3), spheres of atoms about any center point (see 3.1.6), and rectangular boxes of atoms centered on any point (see 3.1.7). Duplicate entries of the same atomic position are prevented by the program. The content of the ATOMS list is printed on the monitor output tape after each 400 series instruction.

3.3.5.1 Instructions 401 and 411, Atom Designator Run Add and Atom Designator Run Eliminate. — These instructions can contain: (a) atom designator codes (ADC) for a single atom, (b) atom designator runs (ADR) for several atoms in a run, (c) blank fields (except between the two entries of a run), and (d) any combinations of (a), (b), and (c). Since up to 19 Format No. 1 continuations are possible per instruction, up to 70 runs can be made per instruction and an unlimited number of instructions can be used. The ATOMS list, however, will only accept the first 500 atoms.

Columns

1–3	Blank or 1 (depending on what follows)
4–9	401 or 411
10–18	
.	
.	
64–72	As described above

3.3.5.2 Instructions 402 and 412, Sphere of Enclosure Add and Sphere of Enclosure Eliminate. — These instructions allow the user to build or modify the subject by specifying the contents (complete, partial, or vector screened, see 3.1.6) of a sphere of enclosure about any addressable point. For instruction 402, the contents of the spheres are *added to* the atom list except for positional duplications, which are omitted. In the 412 instructions, all points in the spheres are *eliminated from* the atoms list if they are present in that list. The instructions call subroutine SEARCH, and the instruction input details are identical to those of instructions 101 and 102 (see 3.3.2.1) except for the instruction number. In the monitor output, only the ATOMS list atom designator codes are printed and not the coordinates and interatomic distances. If the origin atoms on which the spheres of enclosure are centered are to be saved, the target atom number run (Tar. ANR) must contain this atom number. Furthermore, if vector

search code cards of Format No. 2 are used, one of them must satisfy the intra-atom null vector for the origin atom in order to retain it.

3.3.5.3 Instructions 403 and 413, Box of Enclosure Add and Box of Enclosure Eliminate. — These instructions allow the user to build or modify the subject by specifying the contents (complete or partial but *not* vector screened, see 3.1.7) of a box of enclosure about any addressable point (or atom number run of addressable points). The three axes of the box are parallel to the three base vectors of the reference Cartesian system, and the *semidimensions* of the box are specified on the instruction card. If an orientation of the box different from the standard orientation (see 3.1.8) is desired, than a 501 or a 502 instruction, or both, should be used before this instruction to reorient the reference Cartesian system. After this instruction has been executed, the reference system can undergo further reorientation as desired for plotting purposes, etc.

As in the case of the sphere of enclosure (see 3.3.5.2), the origin atom on which the box is centered will not be included unless the target atom number run includes the origin atom number. Vector search codes are not used by this instruction. Subroutine SEARCH is used by this instruction, and the instruction input details are similar to those described in 3.3.2.1 except that D_{\max} is replaced by the semidimension $a/2$ of the box and the following fields on the card are used to specify the other two semidimensions $b/2$ and $c/2$. One must use caution in choosing the box dimensions so that the atom table does not overflow.

Columns

1–3	Blank
6–9	403 (or 413)
10–18	Origin ANR (see 3.3.2.1)
19–27	
28–36	Target ANR (see 3.3.2.1)
37–45	
46–54	$a/2$
55–63	$b/2$
64–72	$c/2$

3.3.5.4 Instruction 410, Clear Atoms List. — This instruction clears the atoms list to zero. When the program is first entered the list is automatically set to zero.

3.3.6 Orienting Instructions (500 Series). — This series of instructions orients the reference and working Cartesian systems (see 3.1.8). Each time the reference system is redefined with a 501 or rotated with a 502, the working system is automatically made coincident with the reference system. The working system can be displaced from the reference system by rotating about an axis of the reference system with a 503 instruction. The working system is always positioned by a rotation from the reference system and does not depend on the previous working system orientation. After each 500 series instruction, the base vectors of the relevant Cartesian system are printed out. These vectors are based on the triclinic coordinate system. The postfactor transformation matrix for converting from triclinic coordinates to

Cartesian coordinates is also printed out. The inverse transformation matrix may be formed by placing the three base vectors together in row vector form.

3.3.6.1 Instruction 501, Reference Cartesian System Assignment. — Any Cartesian coordinate system is based on three orthonormal base vectors and an origin point. The origin point in the model (ORGN) is specified with an atom designator code. The three orthonormal base vectors can be described by two non-collinear vectors, and OR TEP provides the two following separate techniques for performing this operation, using vector cross products of the two vectors \mathbf{u} and \mathbf{v} .

	Type A	Type B
Base vector 1 (x axis)	\mathbf{u}	\mathbf{u}
Base vector 2 (y axis)	$\mathbf{u} \times \mathbf{v}$	$(\mathbf{u} \times \mathbf{v}) \times \mathbf{u}$
Base vector 3 (z axis)	$\mathbf{u} \times (\mathbf{u} \times \mathbf{v})$	$\mathbf{u} \times \mathbf{v}$

The reference system x and y axes will parallel the plotter x and y axes, and the origin point ORGN will lie in the plane of the plotter. The viewer will be looking into the z axis vector of the coordinate system from a distance VIEW in inches (see 3.3.4.1) directly above the origin point.

Columns		Effective Primer Constant
1–3	—	—
6–9	501	—
10–18	ORGN(ADC)	055500
19–27 28–36	Vector \mathbf{u} (VDC)	055500 065500
37–45 46–54	Vector \mathbf{v} (VDC)	055500 056500
55–63	—	—
64–72	0 = Type A, > 0 = Type B	1

3.3.6.2 Instruction 502, Reference Cartesian System Rotation. — The crystal model can be given any orientation desired with a series of rotations of the model about the reference system axes. In general, three rotations (e.g., those of an Eulerian system) are sufficient to achieve any orientation, but for convenience an unlimited number of rotations are permitted in the program. In addition, rotations of 120° about the body diagonal of the reference Cartesian system are permitted (this is achieved by a cyclic permutation of reference base vectors).

Each operation requires two fields in the instruction card. For axial rotations, the first field of each pair will have the number 1, 2, or 3 to indicate rotation about the x , y , or z axes of the reference system. The second field will have the rotation angle in degrees for a right-handed rotation of the model about the designated axis (i.e., a positive angle signifies a counterclockwise rotation of the structure with the designated axis pointing toward the reader). The body diagonal rotation is designated by either a (-1)

or a (-2) in the first field to indicate a 120° or a 240° right-handed rotation about the body diagonal, and the second field is blank. A (-3) would rotate the structure completely around and thus not change its previous orientation.

Columns

First Card

1-3	0 (or 1 if continued on next card)
4-9	502
10-18	$1,2,3,-1,-2$
19-27	ϕ_1°
28-36	$1,2,3,-1,-2$
37-45	ϕ_2°
46-54	$1,2,3,-1,-2$
55-63	ϕ_3°
64-72	$1,2,3,-1,-2$

Second Card

10-18	ϕ_4°
.	.
.	.
.	.

If desired, each rotation can be executed with a separate 502 instruction card.

3.3.6.3 Instruction 503, Working Cartesian System Rotation (Stereoscopic Rotation). — The working (minor) Cartesian system is automatically made coincident with the reference system whenever the reference system is redefined with a 501 instruction or rotated with a 502 instruction. To define an orientation of the working system which is not coincident with the reference system we use a 503 instruction, which allows one rotation about one axis of the reference system. Actually any number of successive rotations can be made, but the effect is not cumulative since the starting point for each rotation is always the reference system. Body diagonal rotations are not permitted.

A 503 rotation normally precedes each member of a stereoscopic pair of plots. The rotation is about axis 2 if the stereo pair is to be viewed with the x axis parallel to the observer's interocular line and about axis 1 if the y axis is to be parallel to that line.

Column

1-3	-
4-9	503
10-18	1,2,3
19-27	ω°

3.3.7 Positioning and Scaling Instructions (600 Series). — These instructions are used to direct the placement of the origin point ORGN (specified by instruction 501) onto the drawing (dimensioned by in-

struction 301). In addition the three-dimensional assembly of atoms (chosen by the 400 series instruction) constituting the model is scaled. The atomic centers of the model will then be hanging in space above and below the drawing board correctly positioned to be projected from the eye point described with 301.

3.3.7.1 Normal Modes of Positioning and Scaling. — Several normal modes of operation are available to the user for positioning and scaling the model. Instruction 601 requires the user to supply a complete explicit description of position (x_0, y_0) and scale (SCAL1). At the other extreme, instruction 604 automatically scales and positions the model so that the peripheral projected atom centers will touch two opposite borders and the peripheral atoms in the remaining dimensions will be centered on the drawing. An intermediate mode is available through 602, which provides automatic scaling after explicit positioning. In general this allows only one edge of the model to touch a border. Finally, instruction 603 requires an explicit scale and does automatic centering.

In general the 604 is the easiest and safest one to use, but situations arise in which the user should not relinquish control to the program. For example, if a big illustration is to be drawn piecewise on a small plotter, the user will have to maintain control over the scale, and probably over positioning, so that the partial plots can be fitted together correctly.

A second scale factor SCAL2 is required in connection with the ellipsoid (or sphere) size. It is a dimensionless scale factor ratio used to modify all rms displacement values before plotting equi-probability ellipsoids or spheres. A table of SCAL2 values vs probability is given in Sect. 5.2. The primer constant for SCAL2 is 1.54, corresponding to 50% probability. If the instruction's entry for SCAL2 is 0 or blank, then SCAL2 is not modified by the instruction. The same statement also holds for x_0 , y_0 , and SCAL1. That is, if the instruction entry is zero or blank for any of these, then the value of the constant in memory is not changed. This means that an x_0 or y_0 cannot be entered as exactly zero, so that if, zero is wanted, a small nonzero number should be entered.

Columns	601	602	603	604	Primer Constant
1–3	—	—	—	—	—
4–9	601	602	603	604	—
10–18	x_0	x_0	—	—	15.0
19–27	y_0	y_0	—	—	5.5
28–36	SCAL1	—	SCAL1	—	1.0
37–45	SCAL2	SCAL2	SCAL2	SCAL2	1.54

3.3.7.2 Incremental Modes of Positioning and Scaling. — Additional flexibility is provided through the incremental instructions 611, 612, and 613. These allow the user to “nudge” the model or modify the scale factor (SCAL1), or both, after the parameters have been initially set with a previous 600 series instruction. The 611 instruction adds Δx_0 , Δy_0 to the previous x_0 , y_0 position for the ORGN placement and multiplies the existing SCAL1 by ΔK (except if $\Delta K = 0$, SCAL1 is unmodified). Instruction 612 increments the position and then does an automatic scaling; 613 first increments the scale (by multiplying by ΔK) and then automatically repositions.

A conservative general approach is to follow a 604 with a 611 having $\Delta x_0 = 0$, $\Delta y_0 = 0$ and $\Delta K = 0.9$. This will simply reduce the scale 10% so that there is more space for labels, etc.

Column	611	612	613
1-3	-	-	-
4-9	611	612	613
10-18	Δx_0	Δx_0	-
19-27	Δy_0	Δy_0	-
28-36	ΔK	-	ΔK
37-45	SCAL2	SCAL2	SCAL2

3.3.8 Atom Plotting Instructions (700 Series). — These instructions are concerned with drawing various representations of the atom based on the familiar ball-and-stick molecular model. The ball in the general case is an ellipsoid representing a contour surface of equal probability density. Alternatively, when thermal motion is not being portrayed, the ball can be a sphere of arbitrary dimension. The 700 series also has provision for labeling the atomic site with the corresponding chemical symbol. The instructions in this series draw the "ATOMS list" atoms which project onto the usable part of the drawing area. Atoms found to be out of bounds are bypassed, and a Fault Message (NG = 10) is printed on the monitor output. An atom is out of bounds under the following conditions: (1) if its z coordinate in the scaled reference Cartesian system is greater than $\frac{1}{2}$ the viewing distance, (2) if its center after projection falls outside the limiting boundary of the drawing board, or (3) if the projected center is within $\frac{3}{4}$ of the margin width (BRDR) of a limiting boundary.

An ellipsoid, for graphical purposes in OR TEP, is considered to be composed of ellipses and straight lines. The ellipses are of two types, principal ellipses and boundary ellipses. Relative to the viewpoint, a principal ellipse is further subdivided into a front half and a back, or hidden, half. There are three principal ellipses per ellipsoid, corresponding to the three principal planes. The boundary ellipse is the edge of the ellipsoid as seen from the viewpoint. The front and back halves of the principal ellipses meet at the boundary ellipse. The straight-line segments of the OR TEP ellipsoid are the forward principal axes, reverse principal axes, and octant shading lines.

Figure 3.1 shows various combinations of these elements. It is obvious that certain of these combinations are better representations than others. Instruction 701 generates the 5A model of Fig. 3.1, instruction 702 generates 2A, and 703 produces 3B. Instruction 704 draws the boundary ellipse alone. If an atom is entered as a sphere, the boundary will be circular before projection and slightly elliptical after perspective projection. Instruction 705 allows the user to make up any representation from the basic components.

Chemical symbols up to six alphanumeric characters in length are included with the input structural parameters for each atom. These symbols can be put onto the illustration with one 700 series or several 900 series instructions. The 700 series places the center of the six-character field of each atom in the same position relative to the atom center; the 900 series allows the user to position each symbol individually. The 700 series requires only three parameters as follows: (1) symbol height in inches, (2) parallel

(left-right) offset in inches, and (3) perpendicular (up-down) offset in inches. The parameters refer to the model before projection, and they will change slightly during perspective projection. The parallel and perpendicular offset refer to the exact center of the six-character input field and are relative to the lettering base line set up with the 302 theta rotation. A symbol height of 0 or blank will cause the symbol-drawing routine to be bypassed.

It is possible to vary the thickness of the boundary ellipse line by making it a function of z , the height of the atom from the drawing board. This option is normally used with the 704 (boundary only)

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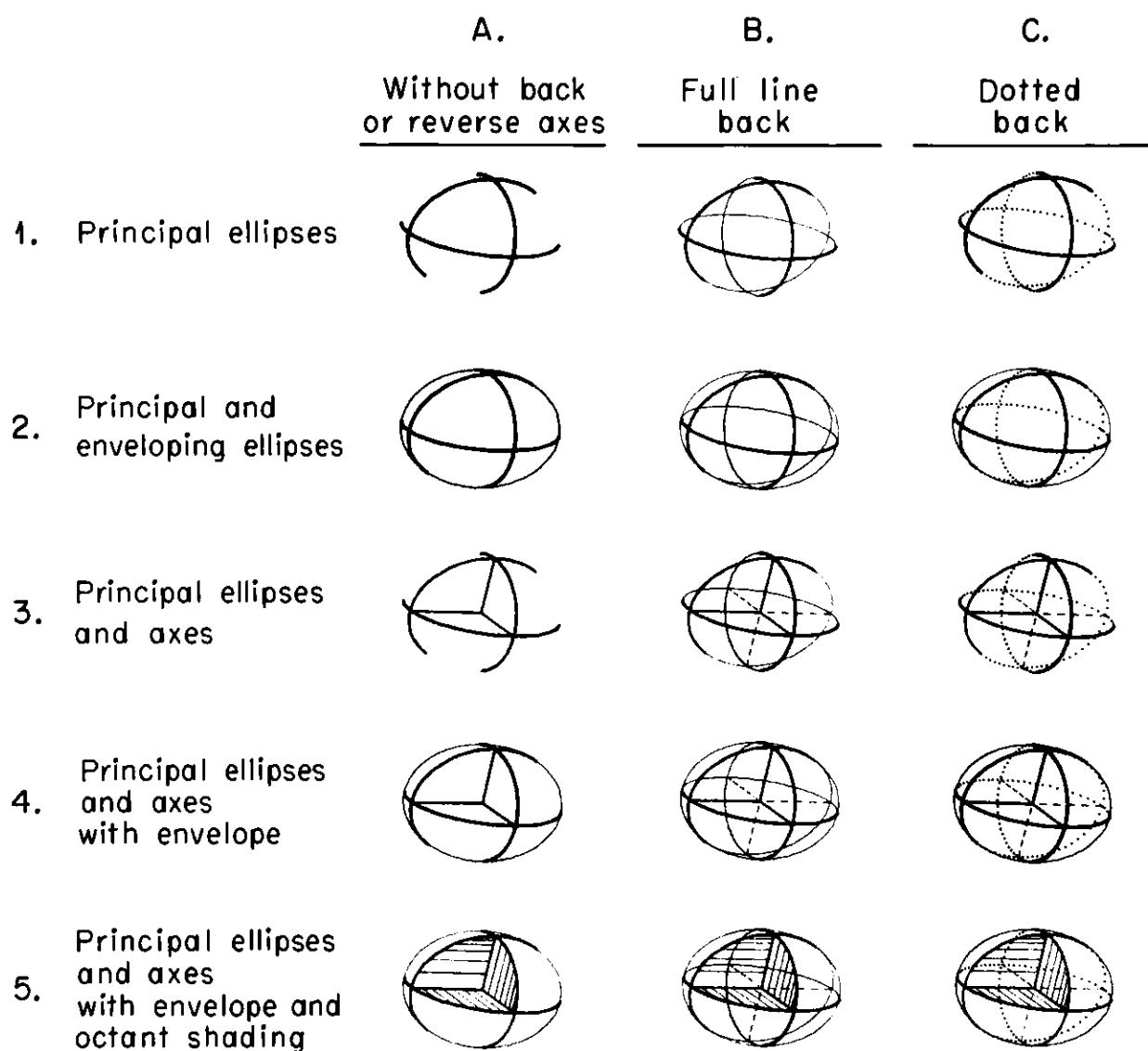


Fig. 3.1. Various Combinations of Ellipsoid Components.

instruction but will work for any 700 instruction. Entries are put in the A_0 and A_1 fields of the instruction continuation card to specify the coefficients of

$$\Delta R(z) = A_0 + A_1 z,$$

where

ΔR is the increase in radial dimension to be added to the width of the single pen line,

A_0 is ΔR for an atom at $z = 0$, and

A_1 is the rate of increase in radial dimension with z .

As an example, assume that the atoms of the scaled model range from 5 in. below to 5 in. above the drawing board and the pen width is 0.2 mm (.008 in.). If we want the closest ellipse boundary to be five times as wide as the farthest, then $\Delta R(-5 \text{ in.}) = 0$, $\Delta R(5) = 0.008 \times (5 - 1) = 0.032 \text{ in.}$; thus $A_0 = 0.016 \text{ in.}$ and $A_1 = 0.0032 \text{ in.}$

The program widens the line by stepping radially in increments of DISP, which is set by primer constant to 0.005 in. A 303 instruction can be used to change DISP if desired.

The monitor output for the 701 through 705 instructions consists of the following:

1. x,y plotter coordinates: the coordinates, in inches, for the projected atom center on the plot, measured from the lower left-hand corner of the limiting boundary. This is the fixed plotter coordinate system with origin point set by the plotter operator.

2. x,y,z working Cartesian coordinates: the coordinates, in inches, for the oriented and scaled atomic model before projection. The x and y axes parallel the plotter x and y axes, and the origin of the system is in the plane of the plotter at the point x_0, y_0 (see 3.3.7) in plotter coordinates. The point ORGN of the scaled model is at this point (see 3.3.6.1).

3. x,y,z triclinic coordinates, in fractions of the unit-cell edges relative to the crystal unit-cell origin.

4. Principal axes of thermal motion, consisting of (a) principal values of root-mean-square displacement and (b) direction cosine for principal vectors relative to the working Cartesian system.

5. The atom designator code and chemical symbol for the atom.

Instructions 711 through 715 are identical to 701 through 705 except that the 710 series suppresses all monitor output except fault messages.

3.3.8.1 Atom Plotting Instructions 701, 702, 703, 704, and 711, 712, 713, 714. —

Columns

First Card

1–3	1 (if boundary retracing is desired; otherwise 0)
4–9	701, 702, 703, 704, 711, 712, 713, 714
10–18	Blank
19–27	Blank
28–36	Blank
37–45	Blank

46-54	Symbol height (in.)
55-63	Perpendicular offset (in.)
64-72	Parallel offset (in.)

Second Card (needed only for boundary retracing)

1-3	Blank
4-9	Blank
10-18	A_0 (in.)
19-27	A_1 (in.)

3.3.8.2 Atom Plotting Instructions 705 and 715. —

Columns

First Card

1-3	1 (if boundary retracing is desired; otherwise 0)
4-9	705 or 715
10-18	NPLANE = 0, no ellipsoid components = 1, boundary ellipse only = 3, principal ellipses only = 4, boundary + principal ellipses
19-27	NDOT (back side of principal ellipses) <0, solid line back side = 0, back side omitted = 3, 4 dots on back side = 4, 8 dots on back side = 5, 16 dots on back side = 6, 32 dots on back side
28-36	NLINE (forward principal axes and shading) = 0, no forward axes or shading = 1, forward principal axes only = N, forward axes + (N - 1) line shading
37-45	NDASH (dashed reverse principal axes) = 0, no reverse axes = N, dashed reverse axes with N dashes
46-54	Symbol height (in.)
55-63	Perpendicular offset (in.)
64-72	Parallel offset (in.)

Second Card same as 701

3.3.9 Bond Plotting Instructions (800 Series). — The bond plotting instructions are grouped into two general types, explicit and implicit, depending on how the bonds are specified. Explicit bonds require a vector designator code (see 3.1.2) for each bond. Implicit bonds make use of vector search codes (see 3.1.5) to find pairs of atoms from the ATOMS array set up by the 400 series instructions.

There are two types of bonds that can be drawn, stick bonds and line bonds. The line bond is a very crude, but rapid, method useful in drawing preliminary illustrations. It is constructed by placing centered symbols (e.g., +, \times , *, etc.) on the two atom sites and drawing a single straight line between them. Line bonds are always specified implicitly (803, 813 instructions).

The more elaborate bond is the stick bond, which could also be called a conical bond because of its accentuated perspective taper.⁸ Each end of the bond intersects either (1) an ellipsoid or (2) an enveloping cone (tangent cone) which has its apex at the viewpoint and is tangent to an ellipsoid. In general, the ellipsoid intersection is automatically used if the axis of the bond intersects the ellipsoid at a point which is visible to the viewpoint; otherwise, the tangent cone intersection is used, so that the bond appears to terminate at the boundary of the ellipsoid. However, the user can specify that the ellipsoid intersection always be used in order to make the skeleton type model (e.g., 3B of Fig. 3.1) appear even more transparent. The radius of the stick bond and the number of lines which are used to draw the bond are specified by input parameters.

Bond-distance labels can be drawn automatically with stick bonds, but not with line bonds. The bond-distance label numbers are in Angstrom units to one, two, or three places past the decimal point. The bond labels on the illustration will have their base lines parallel to the stick bonds and will be right side up for the viewer. The height of the label in inches and the perpendicular offset distance for the center of the label relative to the center of the bond are parameters to be specified by the user. With the present primer constant for FORE, if the sine of the angle between the bond and the mean viewing vector is greater than 0.5, the lettering is done in perspective along the bond. When the sine of the angle is less than 0.5, the perspective lettering would be excessively foreshortened. The lettering is then made parallel to the plane of the drawing with its base line parallel to the projected bond. Different lettering heights and different perpendicular offset distances can be assigned to the perspective and nonperspective bond-distance labels.

All bond parameters are input with Format No. 2 trailer cards (see 3.3.1). The bond parameters are as follows:

1. Bond type (for stick bond) is designated by an integer NBOND, where $-5 \leq \text{NBOND} \leq 5$. The negative integers denote that both ends of the bonds terminate at the ellipsoids. The positive integers denote bonds ending either at the ellipsoid or the tangent cone, as described previously in this section. An entry of zero draws no bond. A magnitude of 1 for NBOND produces two lines, one for each bond edge, 180° apart in the plane normal to the bond axis. Lines are drawn 90° , 45° , 22.5° , or 11.25° apart for NBOND magnitudes of 2, 3, 4, or 5, respectively. The back side of the bond is not drawn. Representative samples are shown in Fig. 6.1.

2. The bond radius (mean value for stick bonds) is in Angstrom units. Values between 0.01 and 0.06 Å usually give good results. Any positive value may be used as long as it is smaller than the scaled ellipsoid minimum semidimension. The bond radius is not changed by the ellipsoid scale factor ratio SCAL2.

⁸The accentuated taper may be increased or decreased by changing the value assigned to TAPER in SUBROUTINE PRIME (see TAPER in sect. 4.5).

3. The height of perspective labels for bond distances is entered as zero if no bond distances are to be labeled. Positive values denote the lettering height in inches before projection.
4. The perpendicular offset for bond distance perspective labels (in inches) pertains to offset of the center of the distance label relative to the center of the bond.
5. The height of regular labels for bond distances is entered as zero if no bond distances corresponding to foreshortened bonds are to be drawn. Positive values give the lettering height in inches before projection.
6. The perpendicular offset for bond-distance regular labels has the same definition as parameter 4 above.
7. The significant digits indicator is -1, 0, or 1, denoting bond distance labels with one, two, or three digits, respectively, after the decimal place.

Instructions 801, 802, and 803 differ from 811, 812, and 813 only in the monitor output listing. The second group has no output except error messages. The first group lists: (1) plotter coordinates in inches, (2) scaled Cartesian coordinates (in inches) of atom before projection, and (3) triclinic crystal coordinates for the atoms of each bond. The interatomic bond distance in angstroms is also listed. If an atom of a bonded pair is out of bounds, a fault message (NG = 10) is printed on the monitor output. If the bond is hidden and cannot be drawn, fault message NG = 14 is printed. Fault NG = 13 signifies that an imaginary intersection was found with a bond radius larger than the ellipsoid semidimension.

3.3.9.1 Instructions 801 and 811, Explicit Stick Bonds. — The only entry on the instruction card is the instruction number. A Format No. 2 trailer card is required with the fields specified under column 801 in Table 3.1 properly filled in. The bonds are described with two atom designator codes for each bond. The two atom designator codes for a bond must be in adjacent fields, but blank fields can be inserted between the different bonds. Since there are seven fields available per card, it is a good idea to use only two, four, or six of them so that the card sequence within the instruction (other than first and last cards) will be unimportant.

3.3.9.2 Instructions 802 and 812, Implicit Stick Bonds. — All parameters are input with Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the instruction number.

3.3.9.3 Instructions 803 and 813, Implicit Line Bonds. — All parameters are input with Format No. 2 trailer cards (see Table 3.1). The centered symbol placed on a given atom will be the centered symbol whose calling number corresponds to the atom number modulo 10 (see Fig. 4.2).

3.3.10 Label Plotting Instructions (900 Series). — The 900 series allows the user to plot general titles up to 72 characters in length, chemical symbols up to 6 characters long, bond length labels, and centered symbols. The bond length labels can have two decimal places before the decimal point and one, two, or three places after the decimal point. The 700 and 800 series instructions can plot chemical symbols and bond length labels, but it is often desirable to position certain labels individually with the 900 series.

General titles and bond length labels can be drawn either in perspective or parallel to the plane of the drawing. Chemical symbols and centered symbols are always drawn parallel to the plotter plane.

Instructions 913 through 916 are for perspective lettering, and instructions 901 through 909 produce regular lettering.

Two vectors, the upright vector and the base-line vector, are needed to describe a lettering plane. In OR TEP the upright lettering vector is always parallel to the plane of the drawing. For perspective lettering the base-line vector is a general vector in three dimensions. In the nonperspective case the base-line vector is either along the projection of a general vector or along the vector (in the plane of the plotter) which is oriented with 302 title rotation instruction (theta base line). If theta (set by 302) is zero, then the theta base-line vector is along the plotter positive x axis.

The exact center of the label is always referred to when specifying the position of the label. The program goes through the following steps to position the center point of the label onto the drawing. (1) A point P_1 is found which is either the position of atom A or the mean of two atom positions (atom A and atom B). The atom A position is used if no atom designator exists in the atom B field of the instruction card. (2) A point P_2 is found by (a) translating from P_1 along the base-line vector for the distance specified by *parallel offset*, then (b) translating along the upright vector by the *perpendicular offset* distance. (3) A point P_3 is found by projecting P_2 onto the plane of the plotter. (4) If the *x edge reset* is > 0 , then *x* is reset to this value. If *x edge reset* is < 0 , *x* is reset to the positive *x* plot boundary minus $|x \text{ edge reset}|$. No resetting is done if *x edge reset* is zero. The *y* parameter is handled in the same manner with *y edge reset*.

The format for the entire 900 series is as follows:

Columns	
1–3	Blank or 3 (or 1 if second card is needed)
4–9	Instruction number
10–18	Designator for atom A
19–27	Designator for atom B (or blank)
28–36	<i>x edge reset</i> (in.)
37–45	<i>y edge reset</i> (in.)
46–54	Lettering height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
Second Card (if needed)	
1–3	Blank
4–9	Blank
10–18	Centered symbol number (0–14)

3.3.10.1 Instruction 901. — A nonperspective chemical symbol with theta base line is drawn using the chemical symbol for atom A.

3.3.10.2 Instruction 902. — A nonperspective title with theta base line is drawn. The title must be entered with the instructions on a Format No. 3 trailer card. The title should be centered about columns 36–37 of that card.

3.3.10.3 *Instructions 903 and 913.* – A general vector title is drawn with nonperspective lettering for 903 and perspective lettering for 913. The general vector is from atom A to atom B. The title is entered as described for 902 (see 3.3.10.2 above).

3.3.10.4. *Instructions 904, 905, 906, 914, 915, and 916.* – These are instructions for general-vector bond-length labels. The first three are for nonperspective lettering with one, two, and three places after the decimal point; and the last three are for the corresponding bond-length labels with perspective lettering. The general vector is from atom A to atom B. Note that the sense of the vector is important in order to have the label right side up.

3.3.10.5 *Instructions 908 and 909.* – These instructions are for centered symbols. With 908 the pen is up while moving to the position where the centered symbol is to be drawn, but *with 909 the pen is left down.* The centered symbol is one of the 15 listed for the CalComp SIMBOL routine (the misspelling of “symbol” is intentional). The symbol number must be in the range 0–14.

3.3.11 **Saved Sequence Instructions (1100 Series).** – It is often desirable to repeat a sequence of instructions one or more times with other instructions inserted between the repetitions. The 1100 series allows the user to do this without the necessity of putting in duplicate sequences of instruction cards. It is not an elaborate looping device, but it does give additional flexibility to the system.

The three instructions in this series are to start the saved sequence (instruction 1101), terminate the saved sequence (instruction 1102), and execute the saved sequence (instruction 1103). All instruction cards and their trailer cards between the 1101 and 1102 instructions are executed and saved on a magnetic scratch tape. A 1103 instruction rewinds this scratch tape and repeats all the instructions stored there before another instruction is read from the monitor input. There are no parameters to be entered with the 1100 series instructions.

3.3.12 **Job Termination Instructions (Negative Series).** – A (-1) instruction terminates the job and exits via SUBROUTINE EXIT.

A (-2) instruction reinitializes the whole program and starts over with another structure from the title card on. As many structures as desired may be run in sequence in this manner before exiting with a (-1) instruction. Note that the 201 instructions should occur only once and should not be repeated for succeeding jobs.

3.4 List of Fault Indicators

Certain errors are checked for in OR TEP, and when one of these occurs, an error message, "FAULT NG = ng ADC m " is written on the monitor output tape. The number NG is explained below. The ADC and m identify the atom code and the instruction involved (if these are relevant). If possible, corrective measures are made by OR TEP and the calculation proceeds; otherwise, the job is terminated by calling SUBROUTINE EXIT.

NG	Subroutine Involved	Fault	Action
1	PRELIM	No sentinel found after reading 48 symmetry cards	Tries to read parameter cards
2	PRELIM	No sentinel found after reading the parameter cards for 200 atoms	Tries to read instruction cards
3	PRELIM	Anisotropic temperature factor coefficients form a matrix which is not positive definite	EXIT after printing out all rms principal values (imaginary ones are negative)
4	ATOM,PAXES	Symmetry operation number is higher than the number of input operations	Omit atom
5	ATOM,PAXES	Atom number is higher than the number of input atoms	Omit atom
6	EIGEN	Null temperature factor matrix or failure in bisection routine	EXIT, after printing out all principal values
7	EIGEN	Eigenvector routine failure due to null vector	EXIT, after printing out all principal values
9	MAIN,SPARE	Unidentified instruction number	Omit faulty instruction
10	BOND,F700	Atom out of bounds	Omit atom
11	F800	No vector search codes	Omit instruction
12	F600	Insufficient number of atoms in ATOMS list	EXIT
13	BOND	Imaginary bond intersection	Omit bond
14	BOND	Hidden (end-on) bond	Omit bond
15	F900	Null vector as base line	Omit label

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

Certain of the numerical procedures¹ used in OR TEP are of a nature somewhat unfamiliar to many crystallographers. These aspects are outlined for the benefit of the reader who may wish to write a similar program or modify the present one.

4.1 Graphic-Computational Methods

These are the techniques used in producing the graphical details of the illustrations.

4.1.1 Drawing Ellipsoids. — Figure 3.1 demonstrates the various ellipsoid graphical representations that can be drawn with OR TEP. The major components in the representations are the three principal ellipses and the boundary (outline) ellipse. The principal ellipses have a front half and a back (hidden) half. The entire boundary ellipse is visible.

An ellipse is approximated by connecting a series of points on the ellipse with straight line segments. Points on an ellipse having a general orientation in three dimensions are computed; then each of these points is projected onto the drawing board for plotting.

The basic algorithm for finding the points along a given general ellipse utilizes the properties of conjugate diameters. Assume that we have the three principal axis vectors $\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3$ of the general ellipsoid and a vector \mathbf{V}_4 from the center of the ellipsoid to the viewpoint. The vector \mathbf{V}_5 normal to the polar plane (see Fig. 4.1), whose pole is the viewpoint, can be obtained from

$$\mathbf{V}_5 = \mathbf{A} \mathbf{V}_4 , \quad (4.1.1.1)$$

where \mathbf{A} is the matrix for the ellipsoid which is defined by

$$\mathbf{X}^T \mathbf{A} \mathbf{X} = d , \quad (4.1.1.2)$$

where d is a constant.

The boundary ellipse is defined by two conjugate vectors, one of which is any vector \mathbf{V}_6 perpendicular to \mathbf{V}_5 and the second is \mathbf{V}_7 , where

$$\mathbf{V}_7 = \mathbf{V}_5 \times \mathbf{A} \mathbf{V}_6 . \quad (4.1.1.3)$$

The assumption made for this boundary ellipse derivation is that the view distance is large compared to the ellipsoid size. Therefore, the boundary ellipse defined above always lies on the diametral polar plane (see Fig. 4.1).

¹For a treatment of the solid analytical geometry involved, the following three books are recommended. The first one is particularly useful.

- J. Heading, *Matrix Theory for Physicists*, chap. 3, pp. 81–106, Longmans, Green and Co., London, 1958.
- B. Spain, *Analytical Quadrics*, Pergamon Press, New York, 1960.
- G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers*, McGraw-Hill Book Company, New York, 1961.

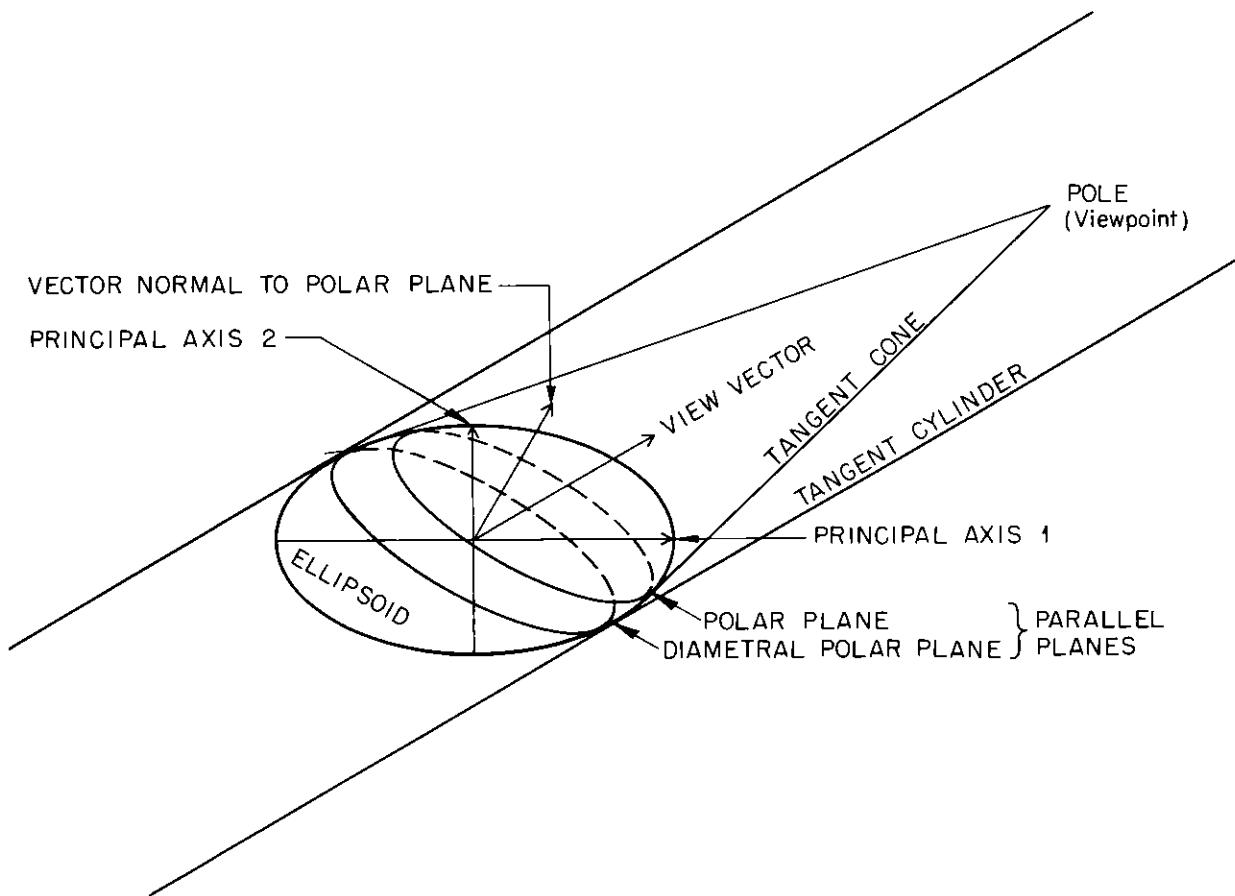


Fig. 4.1. Polar Planes Formed by Tangent Cylinder and Tangent Cone.

A principal ellipse which lies in the plane of the principal axis vectors $\mathbf{V}1$ and $\mathbf{V}2$ will have the third principal axis vector $\mathbf{V}3$ normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector $\mathbf{V}8$ where

$$\mathbf{V}8 = \mathbf{V}5 \times \mathbf{V}3 . \quad (4.1.1.4)$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to $\mathbf{V}8$ and in the principal plane containing $\mathbf{V}1$ and $\mathbf{V}2$ is $\mathbf{V}9$, where

$$\mathbf{V}9 = \mathbf{V}3 \times \mathbf{A} \mathbf{V}8 . \quad (4.1.1.5)$$

After the conjugate vectors have been found, their lengths are adjusted to make them satisfy (4.1.1.2) by letting $\mathbf{X} = s \mathbf{l}$ where \mathbf{l} is a unit vector. Solving for s , we obtain

$$s = [d/(\mathbf{l}^T \mathbf{A} \mathbf{l})]^{1/2} . \quad (4.1.1.6)$$

A conjugate vector pair is expanded into an ellipse by subroutine RADIAL. Since an ellipse is centrosymmetric, the two conjugate vectors and their negatives give us four vectors whose end points lie on the ellipse. By performing a vector sum of two adjacent vectors and dividing the resultant vector components by $\sqrt{2}$, we can obtain an additional vector. After doing this for all adjacent pairs, we then have a total of eight vectors. This process can be repeated as many times as desired except that the scaling constant will be different for each cycle. The constant is described by

$$\text{CONT}(i) = \{2[1 + \cos(\pi/i)]\}^{1/2}$$

where i is the cycle number.

This total process may be thought of as taking a planar radial set of equally spaced unit vectors and performing a deformation and scaling on the space in which it is described. In geometry this deformation is called an affine transformation.

Complete details on drawing ellipsoids can be obtained from the FORTRAN coding of subroutines F700 and RADIAL.

4.1.2 Drawing Bonds. — The major problem in drawing bonds is to obtain the intersection where the bond penetrates the ellipsoid. Three quadrics are used in subroutine BOND to calculate bond intersection. These three are the ellipsoid, the tangent cylinder, and the tangent cone.

The ellipsoid is described in matrix notation as

$$\mathbf{X}^T \mathbf{A} \mathbf{X} = d, \quad (4.1.2.1)$$

where d is a constant and \mathbf{X} is any vector from the center to the surface of the ellipsoid. The matrix \mathbf{A} is 3 by 3 symmetrical with components a_{ij} ($i, j = 1, 2, 3$).

The elliptic cylinder tangent to the ellipsoid and with its axis along z is described by

$$\mathbf{X}^T \mathbf{B} \mathbf{X} = d, \quad (4.1.2.2)$$

where

$$\mathbf{B} = \begin{pmatrix} a_{11} - \frac{a_{13}a_{31}}{a_{33}} & a_{12} - \frac{a_{23}a_{31}}{a_{33}} & 0 \\ a_{12} - \frac{a_{13}a_{32}}{a_{33}} & a_{22} - \frac{a_{23}a_{32}}{a_{33}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (4.1.2.3)$$

and d is the constant used in (4.1.2.1). The tangent cylinder is used when it is necessary to terminate the bond at the boundary of the ellipsoid when a parallel projection is used.

To find the intersection of a cylindrical bond along \mathbf{Vb} with radius r with either the ellipsoid or the tangent cylinder, we proceed as follows:

1. Form a radial set of vectors \mathbf{Vr}_j of length r normal to \mathbf{Vb} .

2. Take a unit vector \mathbf{l} parallel to \mathbf{Vb} and let

$$\mathbf{x}_j = \mathbf{Vr}_j + s \mathbf{l} , \quad (4.1.2.4)$$

where s is a constant to be determined. Substituting in (4.1.2.1) we obtain

$$s^2 \mathbf{l}^T \mathbf{A} \mathbf{l} + 2s \mathbf{Vr}^T \mathbf{A} \mathbf{l} + \mathbf{Vr}^T \mathbf{A} \mathbf{Vr} - d = 0 ; \quad (4.1.2.5)$$

solving for s we get

$$s = \frac{-\mathbf{Vr}^T \mathbf{A} \mathbf{l} + \sqrt{(\mathbf{Vr}^T \mathbf{A} \mathbf{l})^2 - (\mathbf{l}^T \mathbf{A} \mathbf{l})(\mathbf{Vr}^T \mathbf{A} \mathbf{Vr} - d)}}{\mathbf{l}^T \mathbf{A} \mathbf{l}} . \quad (4.1.2.6)$$

The elliptic cone which is tangent to the ellipsoid and which has its apex on the viewpoint can be obtained from the matrix \mathbf{A} and from the vector \mathbf{Vu} which extends from the center of the ellipsoid to the viewpoint. This is performed in the following steps:

1. The ellipsoid is transformed with a rotation matrix to a new Cartesian frame of reference which has the z axis along the view vector \mathbf{Vu} .
2. The tangent cone can now be described as

$$\mathbf{Y}^T \mathbf{C} \mathbf{Y} = 0 , \quad (4.1.2.7)$$

where \mathbf{Y} is a vector originating from the vertex (viewpoint) of the cone and

$$\mathbf{C} = \begin{pmatrix} a_{11} + \frac{a_{13}a_{31}}{K-a_{33}} & a_{12} + \frac{a_{13}a_{32}}{K-a_{33}} & \frac{Ka_{13}}{K-a_{33}} \\ a_{21} + \frac{a_{23}a_{31}}{K-a_{33}} & a_{22} + \frac{a_{23}a_{32}}{K-a_{33}} & \frac{Ka_{23}}{K-a_{33}} \\ \frac{Ka_{31}}{K-a_{33}} & \frac{Ka_{32}}{K-a_{33}} & \frac{Ka_{33}}{K-a_{33}} \end{pmatrix} , \quad K = d/|\mathbf{Vu}| . \quad (4.1.2.8)$$

3. The frame of reference is rotated back to its original orientation with a rotation matrix which is the inverse of the one used in step 1. Note that the origin is now on the viewpoint rather than the ellipsoid center.

To find the length, s , of a vector $s \mathbf{l}$ extending from any point p inside the cone to the surface of the cone we let

$$\mathbf{Y} = \mathbf{Vp} + s \mathbf{l} \quad (4.1.2.9)$$

and obtain from (4.1.2.7)

$$(\mathbf{Vp} + s \mathbf{l})^T \mathbf{C} (\mathbf{Vp} + s \mathbf{l}) = 0 ;$$

then solving for s we obtain

$$s = \frac{-\mathbf{V}_p^T \mathbf{C} \mathbf{l} + \sqrt{(\mathbf{V}_p^T \mathbf{C} \mathbf{l})^2 - (\mathbf{l}^T \mathbf{C} \mathbf{l})(\mathbf{V}_p^T \mathbf{C} \mathbf{V}_p)}}{\mathbf{l}^T \mathbf{C} \mathbf{l}}. \quad (4.1.2.10)$$

The vector \mathbf{V}_p from the vertex to p is formed by

$$\mathbf{V}_p = -\mathbf{V}_u + \mathbf{V}_r,$$

where \mathbf{V}_r is any member of a radial set such as that described for the regular ellipsoid intersection.

4.2 OR TEP Subprograms

The subprograms can be grouped into four functional categories. These can be called Mainstream, Subsidiaries, Arithmetic, and Plotting. The first three categories are coded in a FORTRAN dialect which will compile with either IBM-7090 FORTRAN II or CDC-1604A FORTRAN 63. The plotting routines are generally different for each machine configuration and are usually written in a machine-oriented symbolic language. In general, the standard library plotting routines available at most computing centers can be used with very minor modification.

4.2.1 Mainstream Subprograms. — The first three (PRIME, PRELIM, and MAIN) are the general controlling routines, and the remainder are oriented toward particular OR TEP instructions.

4.2.1.1 PRIME. — This routine "primes the program" by initializing all the "primer parameters" including the magnetic tape logical number assignments.

4.2.1.2 PRELIM. — All calculations concerned with processing (e.g., principal axis transformations) and storing the input crystallographic parameters are performed by PRELIM.

4.2.1.3 MAIN. — MAIN is the controlling routine which decodes the OR TEP instructions. It either executes the command directly or calls the appropriate subroutine which can execute the instruction.

4.2.1.4 F200. — This is the plotter "nursemaid routine" which is controlled through the 200 series instructions. It satisfies the whims and fancies of any particular plotting system control package.

4.2.1.5 F400. — This is the subroutine that executes the 401 and 411 instructions.

4.2.1.6 F500. — This is the subroutine that executes all 500 series instructions.

4.2.1.7 F600. — This is the subroutine that executes all 600 series instructions

4.2.1.8 F700. — This is the ellipsoid plotting routine, which executes all 700 series instructions.

4.2.1.9 F800. — This is the subroutine that executes all 800 series instructions. Bonds to be drawn are found by F800, then drawn by subroutine BOND.

4.2.1.10 F900. — This is the subroutine that executes all 900 series instructions.

4.2.1.11 F1000. — This is a dummy subroutine which is called by the presently nonexistent 1000 series instructions. This series can be coded by the user for any special purpose which may develop.

4.2.1.12 SPARE(NJ). — Further expansion of the instruction list may be done through this dummy subroutine, which is called by any $NJ \geq 12$. NJ = instruction/100.

4.2.2 Subsidiary Subprograms. — 4.2.2.1 **ATOM(ADC,X)**, DIMENSION X(3). — This will find the triclinic coordinates **X** for the atom described by the atom designator code **ADC**.

4.2.2.2 **BOND (ADC1, ADC2, NB)**. — **BOND** is the bond plotting routine to draw a bond, described by Format No. 2 trailer card number **NB**, between atoms **ADC1** and **ADC2**.

4.2.2.3 **DRAW (W,DX,DY,NPEN)**, DIMENSION W(3). — **DRAW** interconnects OR TEP and the plot package. It also prevents the pen from crossing the boundaries. If the indicator **ITILT** in common is zero, the array **W** contains **x** and **y** in plotter coordinates. While perspective lettering is being plotted, **ITILT** ≠ 0; and **W** contains **x**, **y**, **z** in Cartesian coordinates, which will be rotated and projected by **DRAW** to form plotter **x,y** coordinates. **DX** and **DY** are added to the plotter **x** and **y**, respectively, before the plot package is called. **NPEN** = 2 for pen down and 3 for pen up.

4.2.2.4 **ERPNT (ADC,INST)**. — This is the printout routine called when a Fault is found. The arguments identify the atom designator code and the instruction involved in the Fault. The fault indicator, **NG**, is in common.

4.2.2.5 **PAXES (ADC,ITYPE)**. — The covariance (dispersion) matrix for the thermal ellipsoid or its inverse matrix, which is the matrix of coefficients in the quadratic form describing the ellipsoid, is stored in common at **Q** for the atom **ADC**.

ITYPE > 0 for covariance matrix

ITYPE < 0 for ellipsoid quadratic form matrix

|**ITYPE**| = 1 based on triclinic system

|**ITYPE**| = 2 based on working Cartesian system

|**ITYPE**| = 3 based on reference Cartesian system

4.2.2.6 **PLTXY (X,Y)**, DIMENSION X(3),Y(2). — This calculates the plotter coordinates **Y** from the unscaled Cartesian coordinates **X**. The distance to the closest boundary of the plot is placed in common at location **EDGE**.

4.2.2.7 **PROJ (D,DP,X,XO,VIEW,I1,I2,I3)**, DIMENSION D(3,129),DP(2,129),X(3),XO(3). — This routine is used to obtain an array, **DP**, of plotter coordinates from a scaled array, **D**, of points described in Cartesian coordinates. **X**, **XO**, and **VIEW** are parameters involved in the projection, and **I1**, **I2**, **I3** are DO loop parameters for indexing through the array.

4.2.2.8 **RADIAL(ND)**. — Given two conjugate radius vectors of an ellipse in the array **DA** in common, **RADIAL** generates a “radial” array (**D** in common) of points lying on the ellipse. From 8 to 128 points are generated depending on the value of **ND** ($1 \leq ND \leq 5$).

4.2.2.9 **SEARCH**. — Instructions 101, 102, 402, and 403 utilize this routine to conduct an exhaustive (but educated) search to find all points within a sphere or rectangular box. Interatomic distances and angles are also calculated for the 100 series.

4.2.2.10 **STORE**. — This routine stores atoms in (or removes atoms from) the **ATOMS** array. Coordinates in whichever system is in use and the atom designator code are communicated to **STORE** via array **V1** of common.

4.2.2.11 **XYZ(ADC,X,ITYPE)**, DIMENSION X(3). — Coordinates for atom **ADC** are returned in **X**.

ITYPE = 0: triclinic coordinates

ITYPE = 1 or 2: working Cartesian system coordinates

ITYPE = 3: reference Cartesian system coordinates

4.2.3 Arithmetic Subprograms. — **4.2.3.1 Function ARCCOS (X).** — This routine computes θ , the arc cosine of X in degrees; $0 \leq \theta \leq 180^\circ$.

4.2.3.2 AXEQB (A,X,B,N), DIMENSION A(3,3),X(3,3),B(3,3). — This routine solves the matrix equation $\mathbf{A} \mathbf{X} = \mathbf{B}$ for \mathbf{X} . The matrices \mathbf{B} and \mathbf{X} are $(3,N)$ and \mathbf{A} is always $(3,3)$. To invert \mathbf{A} , make \mathbf{B} an identity matrix.

4.2.3.3 AXES (X, Y, A, ITYPE), DIMENSION X(3),Y(3),A(3,3). — This routine provides three orthogonal column vectors in \mathbf{A} , each 1 A long, from the two vectors \mathbf{X} and \mathbf{Y} .

ITYPE > 0: Cartesian system

ITYPE ≤ 0 : triclinic system

|ITYPE| = 1: $\mathbf{A}_1 = \mathbf{X}; \mathbf{A}_2 = (\mathbf{X} \times \mathbf{Y}); \mathbf{A}_3 = \mathbf{X} \times (\mathbf{X} \times \mathbf{Y})$

|ITYPE| = 2: $\mathbf{A}_1 = \mathbf{X}; \mathbf{A}_2 = (\mathbf{X} \times \mathbf{Y}) \times \mathbf{X}; \mathbf{A}_3 = \mathbf{X} \times \mathbf{Y}$

ITYPE = 0: same as type 2 except \mathbf{X} = a crystal axis, \mathbf{Y} = b crystal axis.

4.2.3.4 DIFV (X,Y,Z), DIMENSION X(3),Y(3),Z(3). — This routine performs the vector subtraction $\mathbf{X} - \mathbf{Y} = \mathbf{Z}$. \mathbf{Z} may have the same location as \mathbf{X} or \mathbf{Y} .

4.2.3.5 EIGEN (A,X,B), DIMENSION A(3,3),X(3),B(3,3). — EIGEN determines the three eigenvalues \mathbf{X} and the three column eigenvectors \mathbf{B} of the matrix \mathbf{A} . Indeterminate eigenvectors are replaced by zeros and the Fault indicator NG set to a negative value (eigenvectors are assigned for the indeterminate cases by PRELIM).

4.2.3.6 MM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3). — MM performs the matrix multiplication $\mathbf{A} \mathbf{B} = \mathbf{C}$. The location of \mathbf{C} must be different from \mathbf{A} and \mathbf{B} .

4.2.3.7 MV (A,X,Y), DIMENSION A(3,3),X(3),Y(3). — MV performs the matrix-vector multiplication $\mathbf{A} \mathbf{X} = \mathbf{Y}$. The location of \mathbf{Y} must be different from \mathbf{A} and \mathbf{X} .

4.2.3.8 NORM (X,Y,Z,ITYPE), DIMENSION X(3),Y(3),Z(3). — NORM stores at \mathbf{Z} a vector (not necessarily a unit vector) perpendicular to both \mathbf{X} and \mathbf{Y} . The sense of \mathbf{Z} is that of the vector product $\mathbf{X} \times \mathbf{Y}$.

ITYPE > 0: Cartesian system

ITYPE ≤ 0 : triclinic system

4.2.3.9 TMM (A,B,C), DIMENSION A(3,3),B(3,3),C(3,3). — TMM performs the matrix multiplication $(\mathbf{A}^T \mathbf{B})^T = \mathbf{C}$. The location of \mathbf{C} must be different from \mathbf{A} and \mathbf{B} .

4.2.3.10 UNIT (X,Y,ITYPE), DIMENSION X(3),Y(3). — The vector \mathbf{Y} is made 1 A long and parallel to \mathbf{X} . The vectors \mathbf{X} and \mathbf{Y} may have the same location.

ITYPE > 0: Cartesian system

ITYPE < 0 : triclinic system

4.2.3.11 VM (X,A,Y), DIMENSION X(3),A(3,3),Y(3). — VM performs the vector-matrix multiplication $\mathbf{X}^T \mathbf{A} = \mathbf{Y}^T$. The location of \mathbf{Y} must be different from \mathbf{X} and \mathbf{A} .

4.2.3.12 FUNCTION VMV (X,A,Y), DIMENSION X(3),A(3,3),Y(3). — VMV performs the vector-matrix-vector multiplication $\mathbf{X}^T \mathbf{A} \mathbf{Y} = \text{scalar}$.

4.2.3.13 FUNCTION VV (X,Y), DIMENSION X(3),Y(3). — VV performs the vector-vector multiplication $X^T Y = \text{scalar}$.

4.2.4 Plotting Subprograms for the CalComp Plotter. — The plotting subroutines are taken from the Library routines currently in use at Oak Ridge National Laboratory with the CDC 1604A and the IBM 7090 computers. A CalComp model 580 Magnetic Tape Plotting System is used. The three major routines required are derived from the CalComp subroutines PLOTS, SYMBOL, and NUMBER. The OR TEP modifications are called PLOTS, SIMBOL, and NOMBRE.

4.2.4.1 Subroutine PLOTS. — This is an unmodified CalComp Library routine with two entry points.

a) ENTRY — PLOTS (A, LENGTH, LTNO)

This is the initialization entry for the plotter package and should be used only once in the program. This call must be made prior to usage of any other subroutines in the package.

A is an array which may be used by the plotting package for storing data to be written on the plot tape.

LENGTH is the number of locations in A available to the plotter package.

LTNO is an integer which tells the plotter package the logical tape number of the plotter tape.

In subroutine F200 we have

DIMENSION PLA(2000)

and card F2000170 contains

“210 CALL PLOTS (PLA,2000, LTNO)”

for the CDC 1604A or

“210 CALL PLOTS (PLA(2000),1998,LTNO)”

for the IBM 7090. The reverse storage of common in the IBM 7090 is the reason for the difference.

LTNO is in common and was set to 23 by subroutine PRIME.

An ORTEP 201 instruction directs the execution of this initialization.

b) ENTRY — PLOT (X,Y,IPEN)

This is the basic entry to convey data to the subroutine for plotting. To facilitate the substitution of other plotting routines, ORTEP contains only one instruction (card DRAW0320 in subroutine DRAW) which calls this entry point. All the plotting information passes through DRAW before going to the actual plotting routine PLOT.

X is the abscissa expressed in inches.

Y is the ordinate expressed in inches.

IPEN = 3, the pen will be lifted prior to execution of the movement to the given (X,Y) position.

IPEN = 2, the pen will be lowered to the paper and a straight line will be drawn from the current (X,Y) to the given (X,Y) position.

IPEN = -3, the subroutine will interpret this as being the end of the current plot; and, following movement to the new (X,Y) position, it will set X = 0.0, so that a new origin is established for the following plot (an ORTEP 202 instruction executes this termination procedure).

This subroutine keeps track of current **X** and **Y** positions, and whether or not the pen is in contact with the paper. It stores data in the array **A** provided by the programmer and writes out a record on the specified tape each time the storage area is filled or an end-of-plot call is made. It also generates sequential plot addresses for each plot on the magnetic tape, so that physical plotting of the plots can be done in any order, regardless of the order in which they were placed on tape.

4.2.4.2 Subroutine SIMBOL. — SIMBOL differs from the standard routine SYMBOL in two respects:

1. The input positional parameters specified in the input argument should be an array containing **X**, **Y**, and **Z** in adjacent memory locations. Three-dimensional parameters are required to produce perspective labels. The **Z** parameter is not used by SIMBOL but is transferred to another array that is referenced when SIMBOL calls DRAW.
2. The standard routine SYMBOL calls PLOT directly while SIMBOL calls DRAW which in turn calls PLOT. When perspective labels are used, DRAW will perform a three-dimensional rotation and a projection of the grid points on which the letters are formed, to obtain true perspective. The calling sequence for DRAW is described in 4.2.2.3.

There are two uses of subroutine SIMBOL. The first use is for producing labels, and the second is for plotting one of 15 special centered symbols.

1. ENTRY — SIMBOL (**X(1),X(2),H,BCD,THETA,N**), DIMENSION **X(3)** (note $N \geq 0$)

X(1),X(2) are the **X** and **Y** coordinates of the lower left-hand edge of the first character to be drawn.

X(3) is the **Z** coordinate. It is used only with perspective labeling.

H is the height in inches of the character to be drawn. The width of the character is equal to $\frac{4}{7}$ the height and the character spacing is $\frac{6}{7}$ the height.

BCD specifies the address of an array containing the BCD characters to be plotted.

THETA is the angle in degrees by which the base line of the characters is to be rotated counterclockwise from the positive **X** axis.

N is an integer which specifies the number of characters in the array **BCD** that are to be drawn.

2. ENTRY — SIMBOL (**X(1),X(2),H,NUM,THETA,L**), DIMENSION **X(3)** (note $L < 0$)

X(1),X(2) are the **X** and **Y** coordinates of the center of the symbol.

H is the height of the symbol to be plotted.

NUM is an integer such that $0 \leq NUM \leq 14$ which determines which symbol is to be plotted.

A list of the integers and the symbols generated is shown in Fig. 4.2.

THETA is the angle of rotation as described previously.

L = -1: the centered symbol will be plotted without a line being drawn from the previous (**X,Y**) position.

L < -1: a straight line will be drawn from the previous (**X,Y**) position to the given (**X,Y**) position.

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CENTERED SYMBOLS							
0	:	20		40	-	60	+
1	1	21	/	41	J	61	A
2	2	22	S	42	K	62	B
3	3	23	T	43	L	63	C
4	4	24	U	44	M	64	D
5	5	25	V	45	N	65	E
6	6	26	W	46	O	66	F
7	7	27	X	47	P	67	G
10	8	30	Y	50	Q	70	H
11	9	31	Z	51	R	71	I
12	0	32	□	52	%	72	<
13	=	33	g	53	\$	73	□
14	≠	34	(54	*	74)
15	≤	35	→	55	↑	75	≥
16	!	36	≡	56	↓	76	?
17	□	37	Λ	57	>	77	¤

Fig. 4.2. Characters Available in 1604-A Symbol Routine.

4.2.4.3 Subroutine NUMBER. — This is a subroutine to convert a machine format number to its BCD equivalent and plot it according to a specified format.

NUMBER is different from the usual subroutine NUMBER in that it calls SIMBOL rather than SYMBOL.

ENTRY — NUMBER(X(1),X(2),H,A,THETA,nHFORMAT)

X(1),X(2),H and THETA are described in Sect. 1 of the SIMBOL routine.

A is the address of the floating or fixed point number which is to be plotted.

nHFORMAT is a BCD argument which specifies the manner in which the number is to be converted and plotted.

4.3 Adapting OR TEP to Other Equipment Configurations

Card decks² for ORTEP will be provided free of charge to crystallographers and others who request that the deck be sent to them.

The card deck contains:

1. The FORTRAN source deck with all FORTRAN subprograms arranged alphabetically. An exception is MAIN, which is first in the deck. The deck is set up for compilation by IBM 7090 FORTRAN II. The changes required to compile the deck with CDC 1604 FORTRAN 63 are described in 4.3.1.
2. Either the FAP plotting subroutines for use on the IBM 7090 or the CODAP plotting subroutines for the CDC 1604 will be sent if so requested by the user.
3. Complete binary deck for either the IBM 7090 or the CDC 1604A.
4. Cards for the example figure, cubane.

4.3.1 OR TEP Source Deck Differences for the IBM 7090 and the CDC 1604A. — The following changes should be made to set up the FORTRAN source deck for compilation with CDC 1604 FORTRAN 63.

1. Remove the “*LIST8” and “*LABEL” cards which precede each subprogram.
2. Place a “PROGRAM MAIN” card just before card MAIN0010.
3. Replace card F2000170 with “210 CALL PLOTS (PLA,2000,LTNO).”
4. Replace PRIM0210 with IN = 50,

PRIM0270 with NOUT = 51,

PRIM0280 with NSR = 57,

or with whatever numbers the monitor system requires for Input, Output, and Scratch tapes.

The coding of the plotting routines is completely different for the two systems. In addition, the IBM 7090 plot package contains two subroutines, TRW2 and MSG, which the CDC 1604 package does not have.

²The size of the card deck (3000–5000 cards) is such that it is generally more economical to send the program on magnetic tape. If convenient, the user should send a blank magnetic tape to the author. Card images will be written on that tape in either 200 or 556 bit-per-inch density binary-coded-decimal and the tape returned to the sender. Alternately, the card deck will be sent if desired.

4.3.2 Magnetic Tape Logical Number Assignments. — Logical tape number assignments are made in subroutine PRIME. Four cards are involved in this initialization:

Magnetic Tape Function	Symbolic Name	Primer Constant	Location in PRIME
a) Monitor Input	IN	= 10	PRIM0210
b) Monitor Output	NOUT	= 9	PRIM0270
c) Scratch	NSR	= 11	PRIM0280
d) Plotting	LTNO	= 23	PRIM0240

4.3.3 Plotter Systems Other than the CalComp 580. — In general, only subroutine PLOTS (with entries PLOTS and PLOT) needs to be replaced when a different plotting system is used. This routine is called from only two locations, one in F200 and the other in DRAW. F200 will probably have to be rewritten, and the 200 series instructions may have to be redefined and expanded to accommodate the rules of the new system.

Location DRAW0320 in subroutine DRAW should also be modified to call the new line-drawing routine with the correct argument.

4.3.4 Computing Systems Other than the CDC 1604A and IBM 7090. — Basically, the OR TEP system is designed to be used in a 32 K memory. There are about 7000_{10} unused cells when the system operates with a 32 K word IBM 7090. Consequently, OR TEP would have to be changed considerably to operate in a much smaller memory.

It is hoped that the FORTRAN subprograms will also compile on other machines, but this possibility has not been checked.

If it becomes necessary to replace the machine language subroutines SIMBOL and NOMBRE with completely different routines, the statements calling these routines will also need to be modified.

SIMBOL is called from BOND0450, BOND0470, F7000080, F9001280, F9001310, and F9001450.

NOMBRE is called from BOND2460, BOND2480, BOND2500, F9001380, F9001400, and F9001420.

4.4 Addition of New OR TEP Instructions

Occasions will arise when additional special purpose instructions would be useful. For example, perhaps a cell outline routine would be desirable. (Originally, the 1000 series of instructions were planned for drawing a parallelepiped defined by four general vectors. However, this feature later seemed somewhat redundant and was omitted, since crystal cell outlines can be produced with judicious usage of small dummy atoms and the 800 series instructions.)

The subroutines F1000 and SPARE are intended to be used for additional instructions. All 1000 series instructions call subroutine F1000, which is currently just a dummy routine. Instructions ≥ 1200 call another dummy routine, subroutine SPARE(NJ), where NJ = instruction number/100.

All Arithmetic subprograms (see 4.2.3) and many of the subsidiary subprograms (see 4.2.2) are available for coding these Mainstream subprograms (see 4.2.1).

4.5 Glossary of Symbols in OR TEP Common, with Array Dimensions

	A(9)	Direct crystal cell parameters, a , b , c , $\cos \alpha$, $\cos \beta$, $\cos \gamma$, $\alpha(^{\circ})$, $\beta(^{\circ})$, $\gamma(^{\circ})$.
	AA(3,3)	Metric tensor \mathbf{g} where $g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.
	AAREV(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the reference Cartesian system. AAREV = AA REFV .
	AAWRK(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the working Cartesian system. AAWRK = AA WRKV .
	AID(3,3)	Identity matrix.
	AIN(140)	Array containing the input parameters of the current OR TEP instruction.
	ATOMS(4,500)	Column 1 contains atom designator codes for the atoms which are to be included in the scaling, plotting, bond searching, etc. The other three columns are used for temporary storage of coordinates in any of several coordinate systems.
	BB(3,3)	Reciprocal metric tensor. $\mathbf{BB} = \mathbf{AA}^{-1}$.
P	BRDR	Border width in inches extending inward from plot boundary.
	CD(8,20)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(200)	Chemical symbols for the input atoms.
P	CONT(5)	Constants used in subroutine RADIAL.
	D(3,130)	Array in which three-dimensional points on an ellipse are stored by RADIAL.
	DA(3,3)	Transmits conjugate vectors to RADIAL. Also used for temporary storage.
	DP(2,130)	Array in which two-dimensional points for ellipse are stored after projection.
P	DISP	Displacement parameter for retracing.
	EDGE	Distance in inches from a projected point to the closest boundary. Set in PLTXY.
	EV(3,200)	Root-mean-square displacements for each principal axis of each input atom.
P	FORE	Cosine of critical angle between bond and Cartesian z axis vectors for perspective bond distance labels. At smaller angles the labels, produced from subroutine BOND, are drawn without perspective to prevent excessive foreshortening.
	FS(3,3,48)	Rotation matrices for input symmetry operations based on triclinic system. Used with TS array.
P	IN	Logical number for monitor input magnetic tape.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling ("Tilted Titles").
	KD(5,20)	Part of vector search code array. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
P	LTNO	Logical tape number for magnetic plotting tape.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction (vector search codes).

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	NG	FAULT INDICATOR (see 3.4).
	NJ	Instruction number/100.
	NJ2	Last two decimal digits of the instruction number (instruction = NJ*100 + NJ2).
P	NOUT	Logical number for monitor output magnetic tape.
P	NSR	Logical number for scratch magnetic tape.
	NSYM	Number of input symmetry operations.
	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).
	P(3,200)	Triclinic positional coordinates for the input atoms.
	PA(3,3,200)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 Å long, based on the triclinic system (principal axis vectors).
	PAC(3,5)	A 3×3 matrix produced by subroutine PAXES and made up of three orthonormal principal axis column vectors, based on either the working or reference Cartesian system. Columns 4 and 5 are used in subroutine F700 to duplicate columns 1 and 2 for ease in indexing.
	PAT(3,3)	A matrix produced by subroutine PAXES and composed of three principal axis column vectors each 1 Å long, based on the triclinic system.
	Q(3,3)	A matrix produced by subroutine PAXES. Contains either the dispersion matrix or its inverse, based on either the working or reference Cartesian systems.
	REFV(3,3)	A matrix made up of three orthogonal column vectors, each 1 Å long, based on the triclinic system. This is the base vector triplet for the reference Cartesian coordinate system. The transpose is the postfactor transformation matrix for converting coordinates from the reference orthogonal system to the triclinic system. $\text{REFV}^T = \text{AAREV}^{-1}$.
P	RES(4)	Regulates the resolution of the plotting of a given ellipse as a function of the longest principal axis x in the given ellipsoid of the scaled model.
		$x \geq \text{Res}(1)$ 128-point ellipse
		$\text{Res}(1) > x \geq \text{Res}(2)$ 64-point ellipse
		$\text{Res}(2) > x \geq \text{Res}(3)$ 32-point ellipse
		$\text{Res}(3) > x$ 16-point ellipse
		Res(4) is not used.
	RMS(5)	The rms displacements along the principal axes in arrays PAC and PAT.
P	SCAL1	The scale of the model in inches per angstrom before projection.
P	SCAL2	The scale factor ratio which sets the ellipsoid scale relative to SCAL1. If SCAL2 = 1.54, then the instantaneous position of the atomic center will be within the ellipsoid 50% of the time (50% probability ellipsoid).
P	SCL	$SCL = SCAL1 \times SCAL2$.
P	SYMB(3,3)	A rotation matrix based on the angle THETA which is set by instruction 302.
P	TAPER	The exaggerated bond taper parameter. The top and bottom ends of a bond have radii: RADIUS = 1. ± TAPER * T6 where T6 = cosine of angle between bond and z axis of Cartesian system .

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

P	THETA	Angle in degrees between plotter x axis and lettering base-line vector.
	TITLE(12)	Alphanumeric job title storage.
	TITLE2(12)	Alphanumeric information storage for Format No. 3 trailer card.
	TS(3,48)	Translation vector for each input symmetry operation. Used with FS array.
P	VIEW	Viewing distance in inches.
	VT(3,4)	Perspective title rotation matrix and translation vector. Also used for temporary storage.
	V1(4)	Array to transfer data to subroutine STORE. Also used for temporary storage.
	V2(3) , . . . , V6(3)	Temporary storage.
	WRKV(3,3)	Same definition as for REFV except that this one is for working Cartesian system. $\mathbf{WRKV}^T = \mathbf{AAWRK}^{-1}$.
P	XLNG(3)	Elements (1) and (2) are x and y plot dimensions. Element (3) is not used.
P	XO(3)	Elements (1) and (2) denote the position in plotter coordinates (in inches) where ORGN is placed. Element (3) is not used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.

Note: (P) indicates "prime parameters," which are initialized in subroutine PRIME.

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS

It is convenient to develop the physical significance of the anisotropic temperature factor with the notation and terminology of probability theory rather than with the more familiar Fourier transform theory. The results are, of course, identical regardless of the terminology used. The reason for this choice is that the literature of mathematical statistics and probability theory is somewhat neater and easier to follow. The texts by Wilks,¹ Cramer,² Miller,³ Hamilton,⁴ and Lukacs and Lana⁵ and the handbooks by Burington and May⁶ and Owen⁷ are found to be particularly useful.

5.1 Probability Density Function (pdf) of a Trivariate Normal Distribution

Given three chance variables X_1, X_2, X_3 and S which is a region in X_1, X_2, X_3 space. The probability $P(S)$ that the point (X_1, X_2, X_3) falls in the region S is given by

$$P(S) = \iiint_S \phi(X_1, X_2, X_3) dX_1 dX_2 dX_3. \quad (5.1.1)$$

If the integration is carried over all space, then

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi(X_1, X_2, X_3) dX_1 dX_2 dX_3 = 1. \quad (5.1.2)$$

The function $\phi(X_1, X_2, X_3)$ is called the probability density function (pdf) for the joint distribution of X_1, X_2, X_3 . Using vector notation, we can designate the pdf as $\phi(\mathbf{X})$.

When the distribution is the type said to be normal or Gaussian, the pdf is

$$\phi(\mathbf{X}) = \frac{[\det(\mathbf{M}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp[-\frac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1} (\mathbf{X} - \hat{\mathbf{X}})]. \quad (5.1.3)$$

The matrix \mathbf{M}^{-1} is the inverse of the symmetrical dispersion (variance-covariance) matrix \mathbf{M} , where

$$\mathbf{M} = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13} \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \sigma_2\sigma_3\rho_{23} \\ \sigma_1\sigma_3\rho_{13} & \sigma_2\sigma_3\rho_{23} & \sigma_3^2 \end{pmatrix}.$$

The symbols σ_i^2 represent the second moments or variances about the mean position $\hat{\mathbf{X}}$. The symbols $\sigma_i\sigma_j\rho_{ij}$ are the corresponding covariances and ρ_{ij} are the correlation coefficients.

¹S. S. Wilks, *Mathematical Statistics*, Wiley, New York, 1962.

²H. Cramer, *Random Variables and Probability Distributions*, Cambridge University Press, London, 1962.

³K. S. Miller, *Multidimensional Gaussian Distributions*, Wiley, New York, 1964.

⁴W. C. Hamilton, *Statistics in Physical Science*, Ronald, New York, 1964.

⁵E. Lukacs and R. G. Lana, *Applications of Characteristic Functions*, Hafner Publishing Co., New York, 1964.

⁶R. S. Burington and D. C. May, *Handbook of Probability and Statistics with Tables*, Handbook Publishers, Sandusky, Ohio, 1953.

⁷D. B. Owen, *Handbook of Statistical Tables*, Addison-Wesley, Reading, Mass., 1962.

5.2 Equiprobability Ellipsoids

For a proper normal distribution the quadratic form $(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1} (\mathbf{X} - \hat{\mathbf{X}})$ is positive definite, and a principal axis transformation is possible which will make the cross correlation coefficients $\rho_{ij} = 0$ ($i \neq j$). This transformation is discussed in 5.4. The result of the transformation is the pdf

$$\phi(y_1, y_2, y_3) = \frac{1}{(2\pi)^{3/2} \sigma_{y_1} \sigma_{y_2} \sigma_{y_3}} e^{-Q/2}, \quad (5.2.1)$$

where

$$Q = \frac{(y_1 - \hat{y}_1)^2}{\sigma_{y_1}^2} + \frac{(y_2 - \hat{y}_2)^2}{\sigma_{y_2}^2} + \frac{(y_3 - \hat{y}_3)^2}{\sigma_{y_3}^2}. \quad (5.2.2)$$

The y_i are coordinates based on the Cartesian principal axis system and $\sigma_{y_i}^2$ are the variances along the principal axes, $i = 1, 2, 3$.

The normal probability density function is constant for points on the ellipsoid $Q = C^2$ where C is a constant. The probability that a random point (y_1, y_2, y_3) in the distribution will fall inside the ellipsoid is

$$P(C) = (2/\pi)^{1/2} \int_0^C r^2 e^{-r^2/2} dr. \quad (5.2.3)$$

This result is derived from (5.1.1), (5.2.1), and (5.2.2) by transforming to spherical coordinates.

When $C = 1.5382$, $P = 0.5$ and the corresponding ellipsoid is called the 50% probability ellipsoid. A table of P vs C values is found on page 203 of Owen's *Handbook of Statistical Tables*.⁷ For convenience, that table is reproduced here as Table 5.1.

5.3 Characteristic Function (c.f.) of a Trivariate Normal Distribution

The characteristic function $\Phi(\mathbf{T})$ corresponding to a trivariate distribution $\phi(\mathbf{X})$ is the expected value of $e^{i\mathbf{T}^T \mathbf{X}}$, namely,

$$\Phi(\mathbf{T}) = \int_{-\infty}^{\infty} \phi(\mathbf{X}) e^{i\mathbf{T}^T \mathbf{X}} d\mathbf{X}. \quad (5.3.1)$$

For the trivariate normal pdf (5.1.3) the corresponding characteristic function is

$$\Phi(\mathbf{T}) = \exp [i\mathbf{T}^T \hat{\mathbf{X}} - \frac{1}{2} \mathbf{T}^T \mathbf{M} \mathbf{T}], \quad (5.3.2)$$

where \mathbf{M} is the variance-covariance dispersion matrix described in 5.1 and $\hat{\mathbf{X}}$ is the center of mass of the distribution.

The crystallographic structure factor equation which incorporates general anisotropic temperature factor coefficients is

$$F(\mathbf{h}) = \sum_n f_n(\mathbf{h}) \exp (2\pi i \mathbf{h}^T \hat{\mathbf{X}}_n) \exp (-\mathbf{h}^T \mathbf{B}_n \mathbf{h}), \quad (5.3.3)$$

Table 5.1. Critical Values for Probability Ellipsoids of a Trivariate Normal Distribution^a

P	C	P	C	P	C
0.01	0.3389	0.41	1.3842	0.81	2.1824
0.02	0.4299	0.42	1.4013	0.82	2.2114
0.03	0.4951	0.43	1.4183	0.83	2.2416
0.04	0.5479	0.44	1.4354	0.84	2.2730
0.05	0.5932	0.45	1.4524	0.85	2.3059
0.06	0.6334	0.46	1.4695	0.86	2.3404
0.07	0.6699	0.47	1.4866	0.87	2.3767
0.08	0.7035	0.48	1.5037	0.88	2.4153
0.09	0.7349	0.49	1.5209	0.89	2.4563
0.10	0.7644	0.50	1.5382	0.90	2.5003
0.11	0.7924	0.51	1.5555	0.91	2.5478
0.12	0.8192	0.52	1.5729	0.92	2.5997
0.13	0.8447	0.53	1.5904	0.93	2.6571
0.14	0.8694	0.54	1.6080	0.94	2.7216
0.15	0.8932	0.55	1.6257	0.95	2.7955
0.16	0.9162	0.56	1.6436	0.96	2.8829
0.17	0.9386	0.57	1.6616	0.97	2.9912
0.18	0.9605	0.58	1.6797	0.98	3.1365
0.19	0.9818	0.59	1.6980	0.99	3.3682
0.20	1.0026	0.60	1.7164	0.991	3.4019
0.21	1.0230	0.61	1.7351	0.992	3.4390
0.22	1.0430	0.62	1.7540	0.993	3.4806
0.23	1.0627	0.63	1.7730	0.994	3.5280
0.24	1.0821	0.64	1.7924	0.995	3.5830
0.25	1.1012	0.65	1.8119	0.996	3.6492
0.26	1.1200	0.66	1.8318	0.997	3.7325
0.27	1.1386	0.67	1.8519	0.998	3.8465
0.28	1.1570	0.68	1.8724	0.999	4.0331
0.29	1.1751	0.69	1.8932	0.9991	4.0607
0.30	1.1932	0.70	1.9144	0.9992	4.0912
0.31	1.2110	0.71	1.9360	0.9993	4.1256
0.32	1.2288	0.72	1.9580	0.9994	4.1648
0.33	1.2464	0.73	1.9804	0.9995	4.2107
0.34	1.2638	0.74	2.0034	0.9996	4.2661
0.35	1.2812	0.75	2.0269	0.9997	4.3365
0.36	1.2985	0.76	2.0510	0.9998	4.4335
0.37	1.3158	0.77	2.0757	0.9999	4.5943
0.38	1.3330	0.78	2.1012	0.99999	5.0894
0.39	1.3501	0.79	2.1274	0.999999	5.5376
0.40	1.3672	0.80	2.1544	0.9999999	5.9503

^aReproduced from Ref. 7 by permission of Addison-Wesley Publishing Company, Inc., Reading, Mass. The original caption was "Critical Values for the Spherical Normal Distribution."

where

- \mathbf{h} is a vector giving the Miller indices,
- \mathbf{X}_n is a vector giving the fractional unit cell coordinates of the n th atom,
- \mathbf{B}_n is the anisotropic temperature factor coefficient matrix, and
- $f_n(\mathbf{h})$ is the atom form factor value for atom n .

If a change of variables $\mathbf{T} = 2\pi\mathbf{h}$ is made, then (5.3.3) can be rewritten as

$$F(\mathbf{T}) = \sum_n f_n(T) \exp \left(i \mathbf{T}^T \hat{\mathbf{X}}_n - \frac{1}{2} \mathbf{T}^T \frac{\mathbf{B}_n}{2\pi^2} \mathbf{T} \right). \quad (5.3.4)$$

The scaled anisotropic temperature factor matrix $(1/2\pi^2)\mathbf{B}$ is seen to be identical with the variance-covariance dispersion matrix \mathbf{M} in (5.3.2).

The corresponding crystal space trivariate normal pdf for any particular atom n is

$$\phi(\mathbf{X}) = \frac{[2\pi^2 \det(\mathbf{B}^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp [-\pi^2(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{B}^{-1}(\mathbf{X} - \hat{\mathbf{X}})]; \quad (5.3.5)$$

or if $\mathbf{M}^{-1} = 2\pi^2\mathbf{B}^{-1}$ then

$$\phi(\mathbf{X}) = \frac{\det(\mathbf{M}^{-1})}{(2\pi)^{3/2}} \exp [-\frac{1}{2}(\mathbf{X} - \hat{\mathbf{X}})^T \mathbf{M}^{-1}(\mathbf{X} - \hat{\mathbf{X}})], \quad (5.3.6)$$

which is identical to (5.1.3).

5.4 Principal Axis Transformation

The transformation of anisotropic temperature factor coefficients (for the general triclinic case) to principal axes of thermal motion is discussed by Waser,⁸ Busing and Levy,⁹ and Cruickshank *et al.*¹⁰

The principal axis transformation is necessary to find the thermal-motion probability ellipsoids discussed in 5.2. The principal axes of the matrix \mathbf{M}^{-1} in (5.3.6) are the vectors $\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3$ for which the inner vector product $(\mathbf{y}_i, \mathbf{y}_i)$ has a stationary value subject to the constraint

$$(\mathbf{y}_i, \mathbf{M}^{-1}\mathbf{y}_i) = 1, \quad i = 1, 2, 3. \quad (5.4.1)$$

For the general triclinic crystal system this means that the quadratic form $\mathbf{y}^T \mathbf{G}^{-1} \mathbf{y}$ has a stationary value subjected to the constraint

$$\mathbf{y}^T \mathbf{G}^{-1} \mathbf{M}^{-1} \mathbf{y} = 1, \quad (5.4.2)$$

⁸J. Waser, *Acta Cryst.* **8**, 731 (1955).

⁹W. R. Busing and H. A. Levy, *Acta Cryst.* **11**, 450 (1958).

¹⁰D. W. J. Cruickshank *et al.*, p. 74 in *Computing Methods and the Phase Problem in X-Ray Crystal Analysis*, ed. by R. Pepinsky, J. M. Robertson, and J. C. Speakman, Pergamon, New York, 1961.

where \mathbf{G}^{-1} is the metric tensor with components $a_i \cdot a_j$ and $a_i \cdot a_j$ is the scalar vector product of two of the three unit cell vectors. Introducing the Lagrange multiplier $1/\lambda$ leads to

$$\left[\mathbf{G}^{-1} - \frac{1}{\lambda_i} \mathbf{M}^{-1} \right] \mathbf{y}_i = 0 \quad (i = 1, 2, 3); \quad (5.4.3)$$

premultiplying by \mathbf{M} yields

$$\left[\mathbf{M} \mathbf{G}^{-1} - \frac{1}{\lambda_i} \mathbf{I} \right] \mathbf{y}_i = 0 \quad (i = 1, 2, 3). \quad (5.4.4)$$

Or we can do some additional rearranging and obtain

$$[\mathbf{G} \mathbf{M}^{-1} - \lambda_i \mathbf{I}] \mathbf{y}_i = 0 \quad (i = 1, 2, 3). \quad (5.4.5)$$

Equation (5.4.4) is equivalent to one of the results derived by Busing and Levy, except the λ_i obtained here are the reciprocals of their λ_i because we are doing the principal axis transformation on \mathbf{M}^{-1} while their formulation performs the transformation on \mathbf{M} . The numerical procedure used in OR TEP finds the eigenvalues and eigenvectors of the unsymmetrical matrix $\mathbf{G} \mathbf{M}^{-1}$ in (5.4.4).

6. EXAMPLES OF ILLUSTRATIONS THAT HAVE BEEN PRODUCED WITH OR TEP

Most of the drawings reproduced here were made while OR TEP was under development. Consequently, certain details in the figures are not the same as those produced with the present version of the program. In particular, the lines of shading in the ellipsoid "open octant" are now always evenly spaced.

6.1 Nonstereoscopic Drawings Showing Thermal Motion

The figures in this section have the viewpoint at infinity (parallel projection).

6.1.1 Comparison of Graphical Representations of Thermal Motion. — Figure 6.1 shows the chelation pattern of two citrate molecules related by a twofold screw axis in the crystal structure of magnesium citrate decahydrate.¹ One molecule has "transparent ellipsoids" and the other has "opaque, plugged ellipsoids." Bond types 1, 3, and 4 (see 3.3.9) are illustrated. Note that certain bonds terminate at the ellipsoid boundary while others intersect the ellipsoid. These variables are under the user's control and can be used to advantage for special effects.

Figure 6.2 is another drawing of magnesium citrate decahydrate with the rms magnitudes of displacement along principal axes indicated around the equiprobability thermal ellipsoids.

Figure 6.3 illustrates the same figure with the thermal-motion representation mentioned by Waser,² in which the thermal motion is portrayed by a fourth-degree surface generated by a radius vector with length proportional to the rms component of displacement in the direction of the radius vector. The characteristic peanut shape of this fourth-degree surface is most apparent for atom O₃.

The thermal ellipsoid seems to be the preferred representation, and the present version of OR TEP will draw ellipsoids only.

6.1.2 Thermal Ellipsoids Derived from Independent Sets of Diffraction Data. — Figures 6.4(a) and (b) show the thermal ellipsoids for potassium dihydrogen isocitrate³ obtained from two independent sets of three-dimensional x-ray data (copper K_α data and chromium K_α data). Figure 6.4(a) is presumably a better representation since it is based on a much larger number of measurements. In fact, it is rather surprising that the thermal-motion figures are so similar, considering the limited number of data obtainable with chromium radiation.

6.1.3 Thermal Motion in Molecules Not Related by Crystallographic Symmetry. — Myo-inositol⁴ has two molecules in its crystallographic asymmetric unit. Figures 6.5(a) and 6.5(b) permit a comparison of the two sets of thermal ellipsoids in identical molecular orientations. The hydrogen bonds to neighboring atoms are also indicated. The similarity between the two ellipsoid sets is readily apparent.

¹C. K. Johnson, *Acta Cryst.*, in press (1965).

²J. Waser, *Acta Cryst.* 8, 731 (1955).

³D. van der Helm, J. P. Glusker, C. K. Johnson, J. A. Minkin, N. E. Burow, and A. L. Patterson, *Acta Cryst.*, in press (1965).

⁴I. N. Rabinowitz and J. Kraut, *Acta Cryst.* 17, 159 (1964).

6.2 Stereoscopic Drawings of Crystal Structures

6.2.1 Thermal Ellipsoids Derived from Neutron Studies. — Thermal ellipsoids for hydrogen atoms can be derived from neutron diffraction data. Some recent crystal structure results refined from three-dimensional neutron data are shown here as stereoscopic pairs of perspective projections. The thermal ellipsoid for a hydrogen atom is almost always larger than that of the heavier neighbor atom because of zero-point energy.

6.2.1.1 Chloral Hydrate. — Figure 6.6 features two molecules of chloral hydrate⁵ related by a center of symmetry. The neighboring hydroxyl groups which are involved in hydrogen bonding to the two molecules are also included.

6.2.1.2 Sugars. — A single molecule of sucrose⁶ is shown in Fig. 6.7 with the six-membered glucose ring to the left and the five-membered fructose ring to the right. Two intramolecular hydrogen bonds are drawn between the two moieties. Only one hydroxyl group in the molecule does not form a hydrogen bond; this group has the abnormally large thermal ellipsoid for hydrogen on the left side of the figure.

The thermal motion of a glucose molecule in the α -glucose crystal structure⁷ is illustrated by Fig. 6.8. This figure was drawn with OR TEP by G. M. Brown.

6.2.1.3 Lithium Sulphate Monohydrate. — The inorganic structure lithium sulphate monohydrate has been refined with three-dimensional x-ray data by Larson⁸ and with three zones of two-dimensional neutron data by Smith and Levy.⁹ Figure 6.9 illustrates the characteristic atomic arrangement in that structure. The hydrogen thermal ellipsoids were taken from the neutron analysis and the remainder from the x-ray results. The outstanding feature in this illustration is the large thermal motion of the water molecule, which indicates much looser binding than in the rest of the structure.

6.2.1.4 Potassium Hydrogen Chloromaleate.¹⁰ — This structure contains a centered hydrogen bond. The interatomic bond distances and the surrounding K atoms are also shown in Fig. 6.10, which was drawn with OR TEP by R. D. Ellison and H. A. Levy.

6.2.2 Thermal Ellipsoids Derived from X-Ray Studies. — The examples shown in this section were taken from the literature and from the work of several crystallographers who kindly sent their unpublished results to ORNL to be drawn.

6.2.2.1 Long-Chain Aliphatic Organic Compounds. — Dihydromalvalic acid¹¹ (*cis*,*D,L*-8,9-methyleneheptadecanoic acid) is shown in Fig. 6.11. The thermal motion perpendicular to the chain direction is seen to increase in amplitude toward the nonpolar end of the chain.

⁵G. M. Brown and H. A. Levy, *Abstracts ACA Meeting, Villanova, Pa.*, H-11 (1962).

⁶G. M. Brown and H. A. Levy, *Science* **141**, 921 (1963).

⁷G. M. Brown and H. A. Levy, *Science* **147**, 1038 (1965).

⁸A. C. Larson, *Acta Cryst.* **18**, 717 (1965).

⁹H. G. Smith and H. A. Levy, *Abstracts ACA Meeting, Boulder, Colorado*, 1961.

¹⁰R. D. Ellison and H. A. Levy, *Acta Cryst.*, in press (1965).

¹¹G. A. Jeffrey and M. Sax, *Acta Cryst.* **16**, 1196 (1963).

Figure 6.12 illustrates the thermal motion in the triglyceride beta-tricaprin.¹² The two molecules shown are related by a center of symmetry. Again the amplitude of motion perpendicular to the chain increases toward the end of the chain.

6.2.2.2 Copper Chelation Compound. — The chelation pattern in *bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II)¹³ is demonstrated in Fig. 6.13. The copper atom is on a symmetry center.

6.2.2.3 Large Biological Molecule. — Harunganin,¹⁴ which is a plant pigment, is shown in Fig. 6.14. The pair of "half atoms" at the upper right is an approximation used in the least-squares refinement to correct for either very large thermal motion or disorder which occurs in that part of the crystal structure. The thermal parameters are somewhat questionable since the structure was not refined to convergence. However, the stereogram does permit the molecular configuration to be readily visualized.

6.2.2.4 Abnormal Motion in Cr(III) Acetylacetone. — Dr. Bruno Morosin from Sandia Corporation sent this most unusual example of thermal motion. Cr(III) acetylacetone¹⁵ has three acetylacetone ligands arranged to form an octahedral coordination of oxygens about the Cr atom, as shown in Fig. 6.15. One of the ligands displays very large thermal anisotropy. When a molecular packing diagram such as Fig. 6.16 is viewed, the large displacements are seen to be parallel to the **b** crystal axis. It appears that sheets of these ligands are either disordered or undergoing longitudinal vibration. Morosin has evidence from other diffraction experiments which supports the hypothesis that it is a thermal vibration phenomenon and not static disorder in the crystal.

6.2.3 Crystal Structure Packing Diagrams. — It is often desirable to illustrate the way that molecules pack together in a crystal structure. Sometimes thermal motion can be interpreted on this basis, as was done in 6.2.2.4. In other instances one may be more interested in visualizing the general packing geometry of the crystal structure. Stereograms are very useful for both applications.

6.2.3.1 Potassium Hydrogen Chloromaleate. — A molecule of this structure¹⁶ is shown in Fig. 6.10. Packing diagrams were also drawn by Ellison and Levy and are reproduced here. Figure 6.17 shows the packing of anions about the two types of potassium ions. One coordination polyhedron is an irregular octahedron of oxygen atoms. The other is an irregular 14-hedron having six oxygen atoms and four chlorine atoms at its vertices. Figure 6.18 is a different view of the packing with a larger area included.

6.2.3.2 Packing Diagrams for Inorganic Structures. — The reader may have noticed that most of the illustrations are of organic structures. The reason is that organic molecules are easy to draw. Considerably more planning is required to produce an informative illustration of an inorganic structure.

An approach which is fairly successful is the following:

1. Draw a preliminary stereogram of the contents of a box which encloses somewhat more than one unit cell. Bonds should be drawn in accordance with known interatomic distance ranges. The dimensions

¹²A. J. Mabis and L. H. Jensen, *Abstracts ACA Meeting, Bozeman, Montana*, F-9 (1964) and L. H. Jensen, private communication, 1964.

¹³G. E. Gurr, *Abstracts ACA Meeting, Bozeman, Montana*, K-7 (1964) and private communication, 1964.

¹⁴R. A. Alden, G. H. Stout, J. Kraut, and D. F. High, *Acta Cryst.* 17, 109 (1964).

¹⁵B. Morosin, *Acta Cryst.*, in press (1965) and B. Morosin, private communication, 1964.

for this drawing may be such that the plot can be viewed directly with a stereoscope without photographic reduction.

2. While viewing the preliminary stereogram, pick out the basic structural units and decide on a grouping of these units for the desired figure.

3. Describe the intended subject with whichever technique is the most convenient and draw the new figure. Figure 6.19, potassium perxenate nonahydrate,¹⁶ is an example of an illustration planned in this way. This figure was drawn by J. H. Burns at ORNL.

6.2.3.3 Illustrations of the Contents of a Unit Cell. — A favorite method used by crystallographers is to draw a unit cell outline and the cell contents within that outline. Figure 6.20, which is a stereogram showing lithium α -monodeuteroglycolate,¹⁷ is of this nature. The molecules were kept intact rather than cut off at the cell outline.

6.3 Helical Structures

OR TEP has certain features which facilitate the drawing of nonintegral helical screw models such as those discussed in the field of molecular biology. The Pauling, Corey, and Branson alpha-helix model¹⁸ for protein structure is an example. Figure 6.21 shows the modification of this structure which is present in the synthetic polypeptide poly-L-alanine.¹⁹

¹⁶A. Zalkin, J. D. Forrester, D. H. Templeton, S. M. Williamson, and C. W. Koch, *J. Am. Chem. Soc.* **86**, 3569 (1964).

¹⁷C. K. Johnson, E. J. Gabe, M. R. Taylor, and I. A. Rose, *J. Am. Chem. Soc.* **87**, 1802 (1965).

¹⁸L. Pauling, R. B. Corey, and H. R. Branson, *Proc. Natl. Acad. Sci. U.S.* **37**, 235 (1951).

¹⁹A. Elliott and B. R. Malcolm, *Proc. Roy. Soc. London A* **249**, 30 (1959).

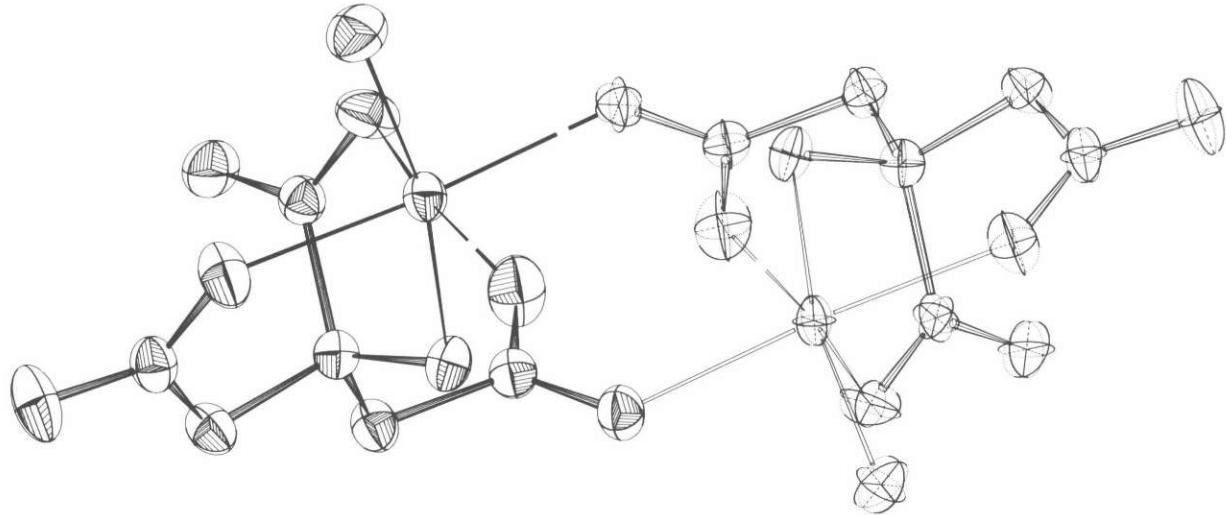


Fig. 6.1. Chelation Pattern Viewed Along a Twofold Screw Axis in the Crystal Structure of Magnesium Citrate Decahydrate. Ellipsoids represent equiprobability surfaces of thermal displacement and contain 65% of the probability distribution.

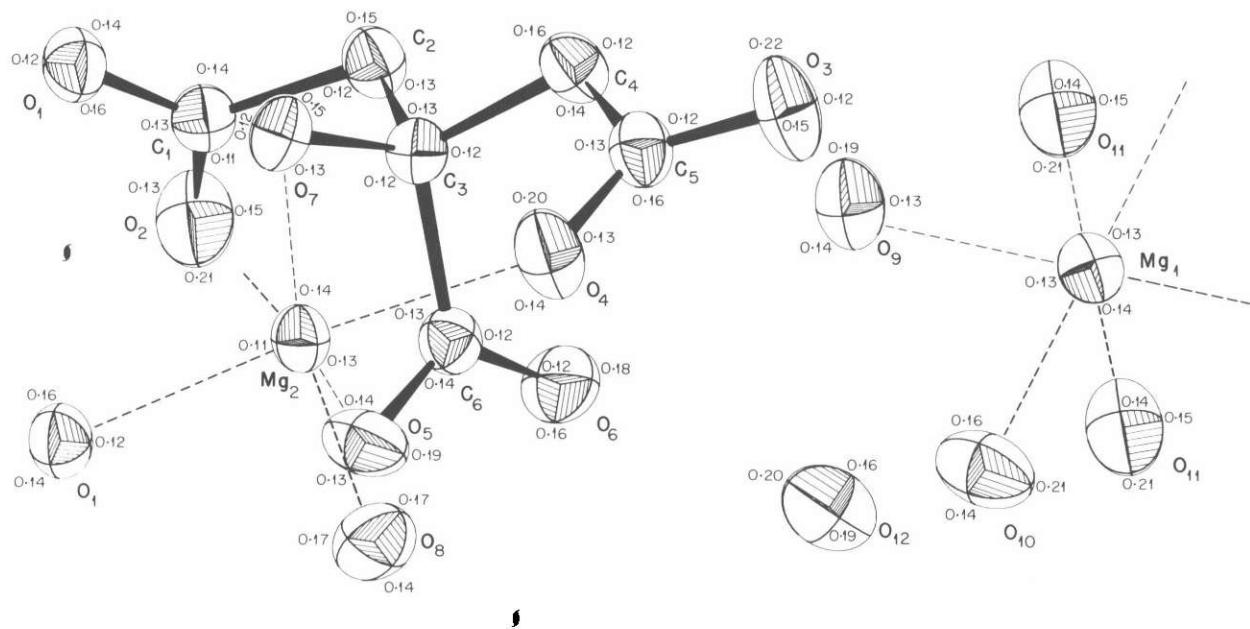


Fig. 6.2. Thermal Ellipsoid Representation for Magnesium Citrate Decahydrate with Principal Values of RMS Displacement in Angstrom Units. Ellipsoids enclose 74% probability. Structure is viewed along *b* axis.

ORNL DWG. 65-2444

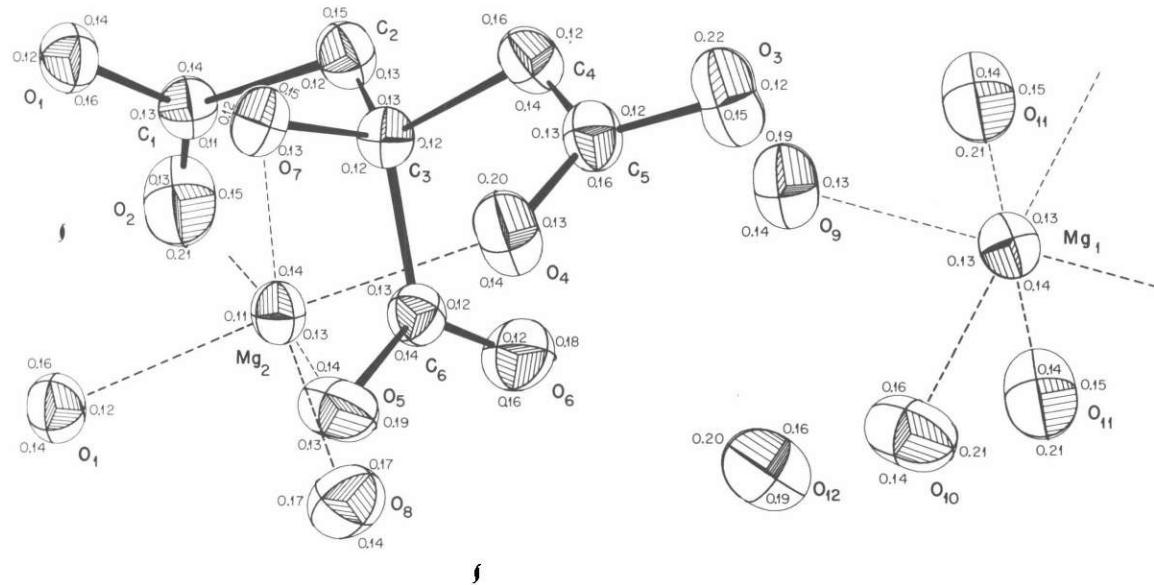


Fig. 6.3. Peanut-Shaped RMS Thermal-Displacement Figure Representation for Magnesium Citrate Decahydrate. Principal values of rms displacement in Angstrom units are indicated around the displacement figures, which are drawn at double scale. Same view of structure as shown in Fig. 6.2.

ORNL DWG. 65-2449

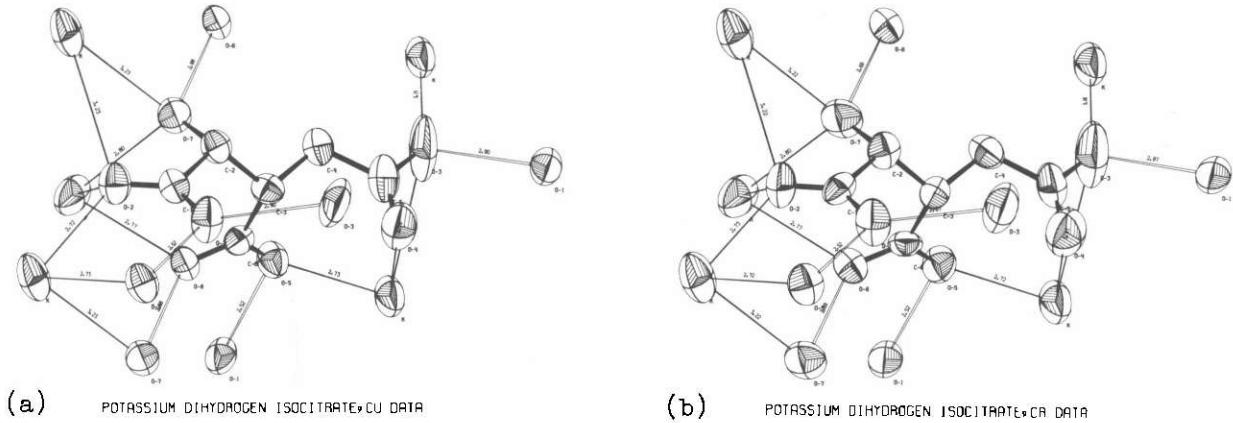


Fig. 6.4. Potassium Dihydrogen Isocitrate with Thermal Ellipsoids Scaled to Include 74% Probability. (a) Results obtained from 1350 three-dimensional copper K_{α} data (disagreement factor 6.5%). (b) Results obtained from 340 three-dimensional chromium K_{α} data (disagreement factor 2.2%). Note: This is not a stereo pair.

ORNL DWG. 65-2450

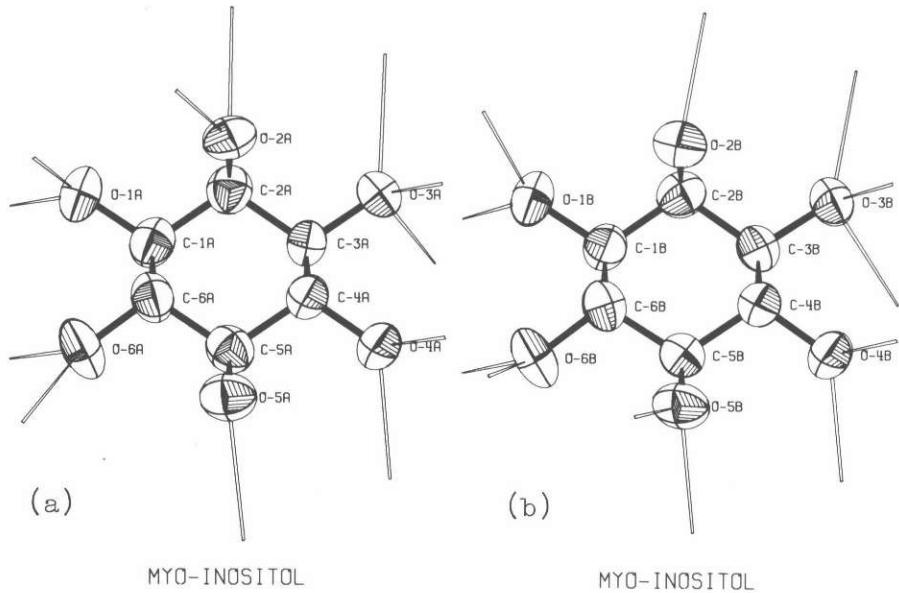


Fig. 6.5. Comparison of Thermal Ellipsoids in the Two Crystallographically Independent Molecules of Myo-Inositol (6.5a and 6.5b). Hydrogen bonding is shown, since this might influence the thermal motion. Ellipsoids are scaled to include 74% probability. Note: This is *not* a stereo pair.

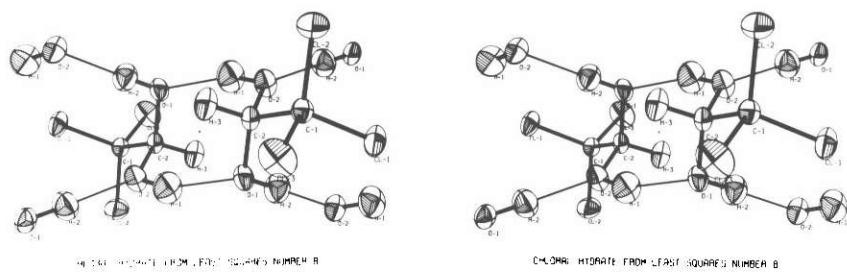


Fig. 6.6. Stereogram (Stereoscopic Pair of Perspective Projections) of Chloral Hydrate Viewed Along the Reciprocal Axis a^* . Two molecules are shown related by a center of symmetry, with the hydrogen bonds connecting them together and to other molecules. Ellipsoids are scaled to include 48% probability.

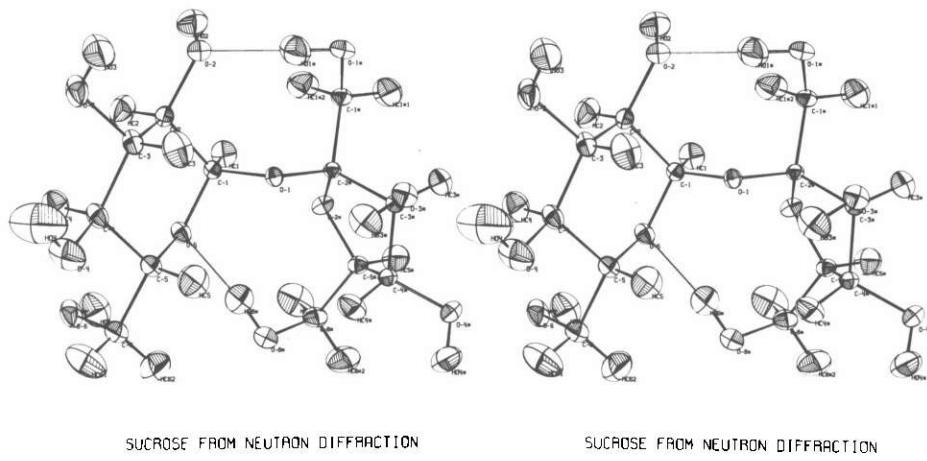


Fig. 6.7. Stereogram Showing the Sucrose Molecule with Thermal Ellipsoids Scaled to Enclose 50% Probability.

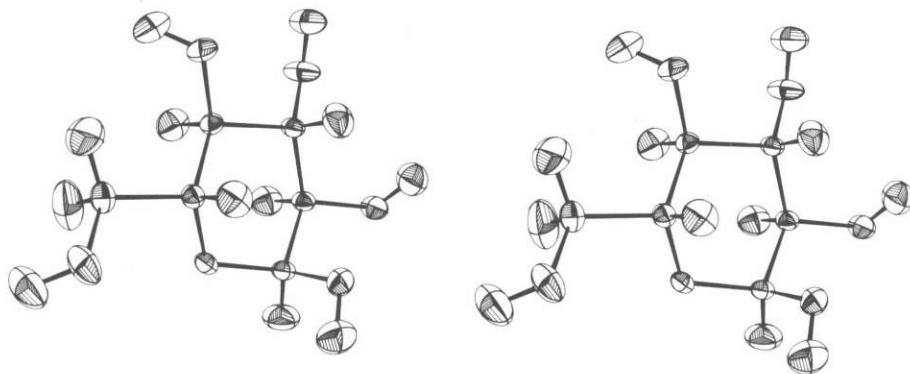


Fig. 6.8. A Molecule of Glucose with Thermal Ellipsoids Scaled to Enclose 50% Probability.

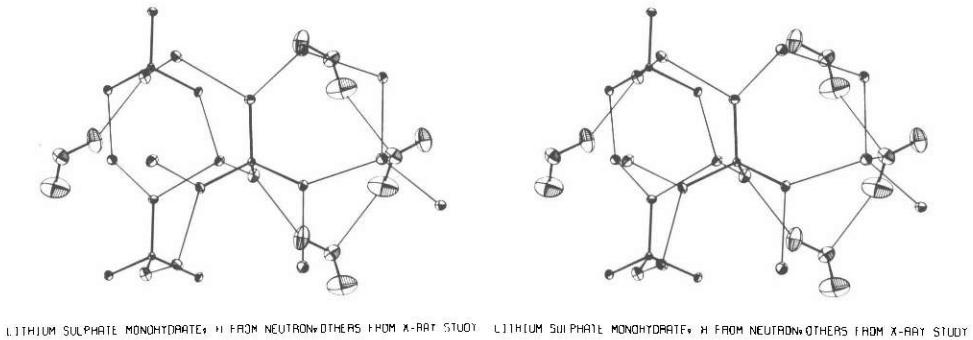


Fig. 6.9. Lithium Sulphate Monohydrate. The lithium ions and sulphate ions are coordinated into a compact network. The structure is viewed along the reciprocal a^* axis. The ellipsoids are scaled to enclose 20% probability.

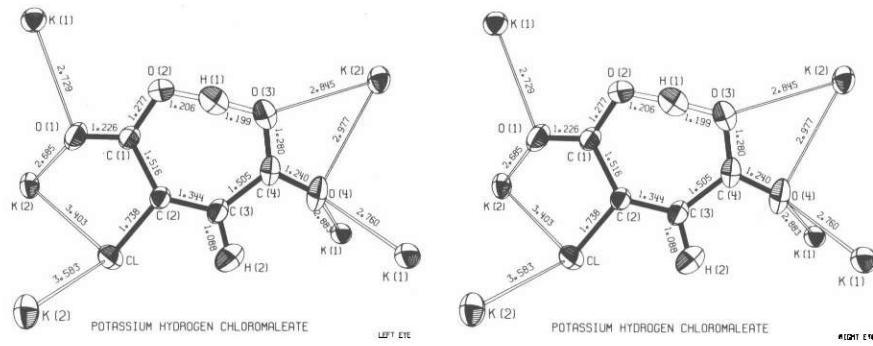


Fig. 6.10. Potassium Hydrogen Chloromaleate. The chloromaleate ion is viewed normal to its own plane. The thermal ellipsoids enclose 50% probability.

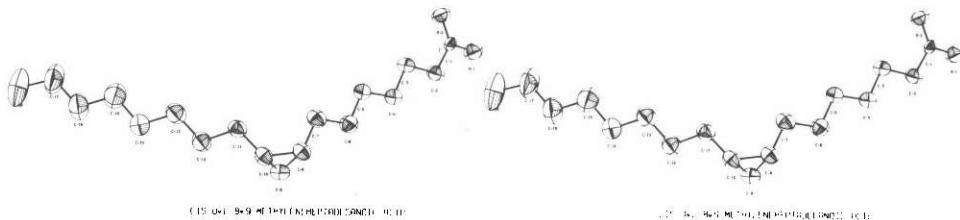


Fig. 6.11. A Molecule of Dihydromalvalic Acid with Thermal Ellipsoids Scaled to Enclose 48% Probability.

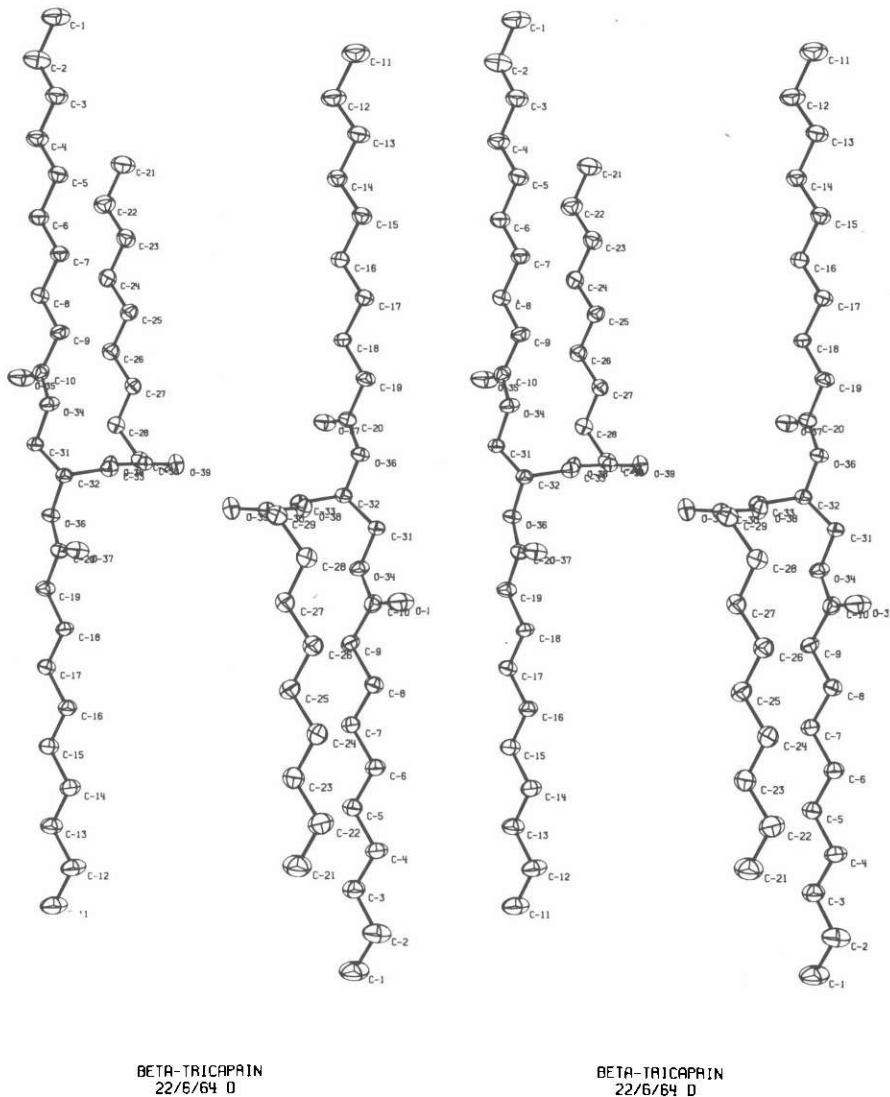


Fig. 6.12. Two Molecules of Beta-Tricaprin Related by a Center of Symmetry. The thermal ellipsoids are scaled to include 30% probability.

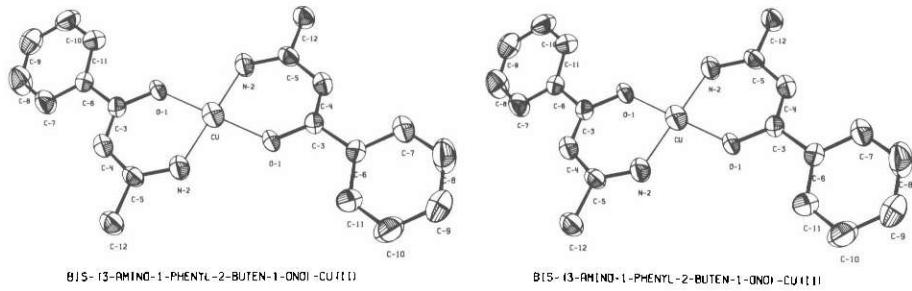


Fig. 6.13. Chelation Complex of *Bis*-(3-amino-1-phenyl-2-butene-1-one)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

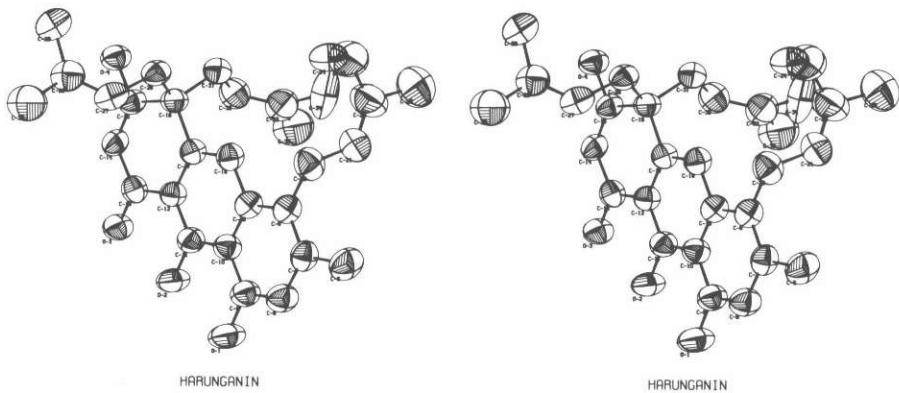


Fig. 6.14. A Molecule of the Plant Pigment Harunganin with Thermal Ellipsoids Scaled to Include 48% Probability.

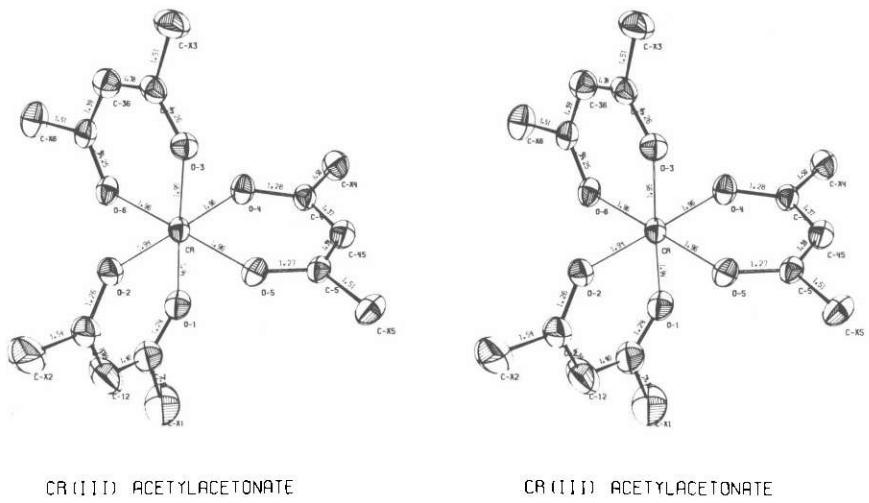


Fig. 6.15. A Unit of *Tris-acetylacetonatochromium(III)* Viewed Along its Threefold Axis of Chemical Symmetry. The thermal ellipsoids are scaled to enclose 20% probability.

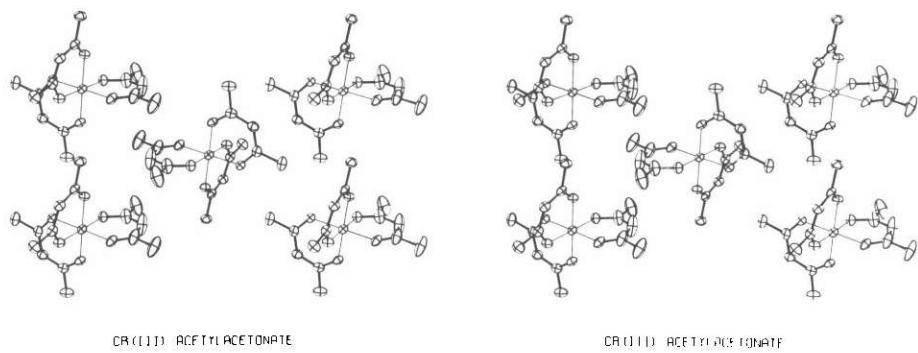


Fig. 6.16. Packing Diagrams for *Tris-acetylacetonatochromium(III)* Viewed Along the Reciprocal Axis c^* . Thermal ellipsoids are scaled to enclose 20% probability.

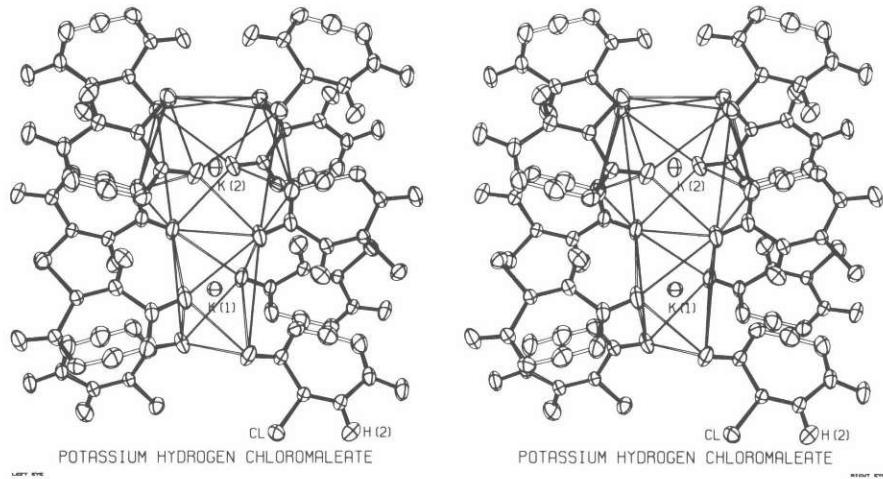


Fig. 6.17. Packing of Chloromaleate Ions Around the Potassium Ions in Potassium Hydrogen Chloromaleate. The edges of the coordination polyhedra are shown. View is nearly along the c axis. Thermal ellipsoids are scaled to contain 50% probability.

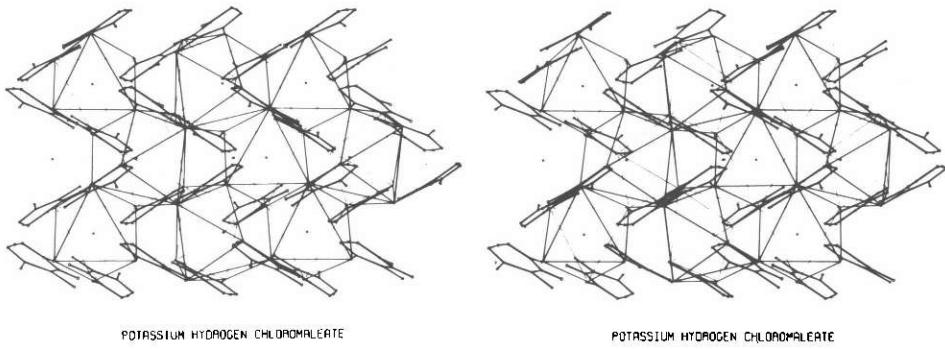


Fig. 6.18. Packing Diagrams for Potassium Hydrogen Chloromaleate. Atoms are represented as small circles. The edges of the coordination polyhedra around the potassium ions are shown. View is nearly along the a axis.

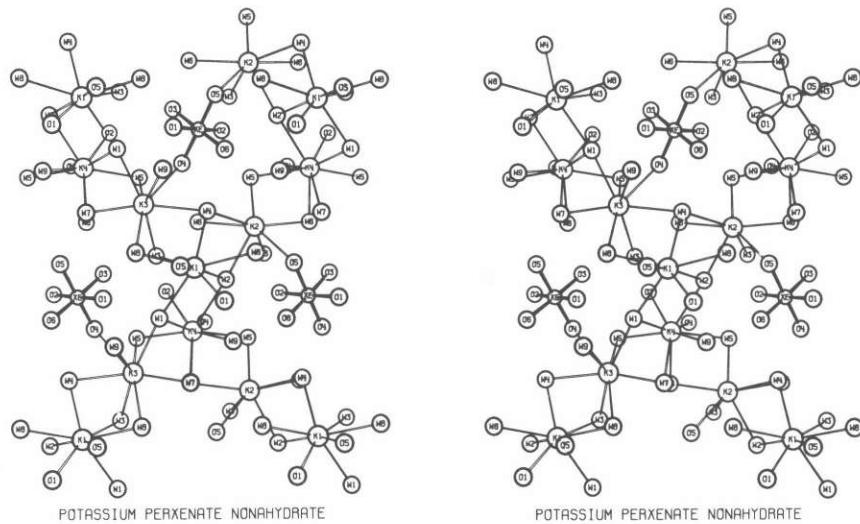


Fig. 6.19. Packing Diagram for Potassium Perxenate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Perxenate Ions. The view is parallel to the a axis. Another layer, related to the present one by a twofold screw axis along a , is needed to complete the structure.

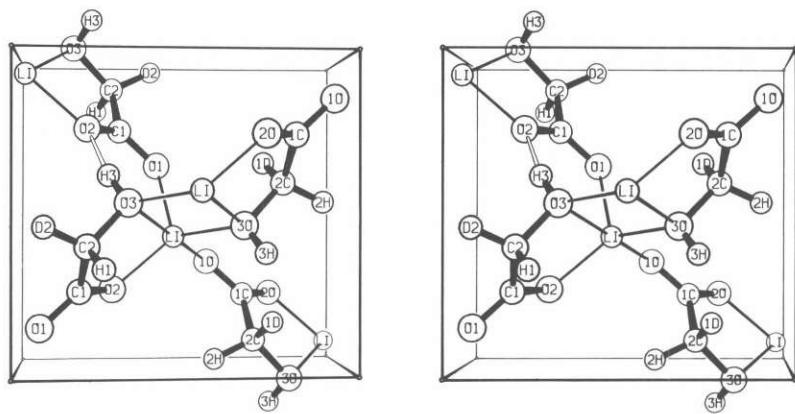


Fig. 6.20. A Stereogram Showing the Unit-Cell Contents of Anhydrous $\text{Li} \alpha$ -monodeuteroglycolate. The unique monoclinic b axis points up in the page and the mean c axis out from the page.

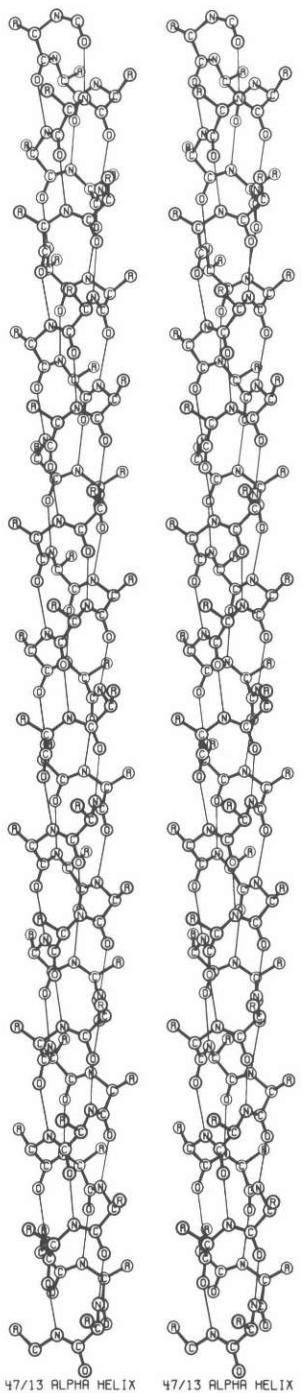


Fig. 6.21. A Stereoscopic Pair of Perspective Projections Showing the Alpha-Helix Which Is Present in Poly-L-Alanine. There are 47 amino-acid residues in 13 turns of the helix. Stereo viewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP

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*LIST8
*LABEL
CMAIN
C ***** OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM *****
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      MAIN0010
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) MAIN0020
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) MAIN0030
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) MAIN0040
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   MAIN0050
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) MAIN0060
      DIMENSION XLNG(3),X0(3),XT(3)                                     MAIN0070
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  MAIN0080
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD MAIN0090
      COMMON NJ,NJ2,NOUT,NSR,NSYM,CRGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL! MAIN0100
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2  MAIN0110
      COMMON V3,V4,V5,V6,WRKV,XLNG,X0,XT                                     MAIN0120
      COMMON V3,V4,V5,V6,WRKV,XLNG,X0,XT                                     MAIN0130
      2 CALL PRIME                                         MAIN0140
C ***** READ JOB TITLE CARD *****
      READ INPUT TAPE IN,4,(TITLE(1),I#1,12)                           MAIN0150
      4 FORMAT(I2A6)                                         MAIN0160
      WRITE OUTPUT TAPE NOUT,6,(TITLE(1),I#1,12)                         MAIN0170
      5 FORMAT(IH01DX,I2A6)                                         MAIN0180
      6 FORMAT(IH11DX,I2A6)                                         MAIN0190
      CALL PRELIM                                         MAIN0200
      WRITE OUTPUT TAPE NOUT,6,(TITLE(1),I#1,12)                         MAIN0210
      ISAVE#0                                           MAIN0220
      GO TO 507                                         MAIN0230
      7 ISAVE#0                                           MAIN0240
C ***** ZERO AIN ARRAY *****
      8 DO 10 J#1,140                                         MAIN0250
      10 AIN(J)#0.                                         MAIN0260
      11 FORMAT(IH04X,I7H((((( INSTRUCTIONI5,6H))))))  MAIN0270
      12 FORMAT(I3,I6,7F9.0)                                         MAIN0280
      13 FORMAT(I3,I6,7E15.8)                                         MAIN0290
      14 FORMAT(IH 9X,7E15.7)                                         MAIN0300
C ***** READ NEW INSTRUCTION CARD *****
      15 NCD#0                                           MAIN0310
      16 NI#N1+7                                         MAIN0320
      17 N2#N1+6                                         MAIN0330
      18 IF(ISAVE)22,18,18                                         MAIN0340
      19 READ INPUT TAPE IN,12,IC,NF,(AIN(I),I#NI,N2)  MAIN0350
      20 IF(ISAVE)24,24,20                                         MAIN0360
      21 WRITE OUTPUT TAPE NSR,13,IC,NF,(AIN(I),I#NI,N2)  MAIN0370
      22 GO TO 24                                         MAIN0380
      23 READ INPUT TAPE NSR,13,IC,NF,(AIN(I),I#NI,N2)  MAIN0390
      24 IF(IC)7,24,24                                         MAIN0400
      25 IF(NI-1)26,26,30                                         MAIN0410
      26 WRITE OUTPUT TAPE NOUT,11,NF                           MAIN0420
      27 NF#NF                                         MAIN0430
      28 IF(NF)28,8,30                                         MAIN0440
      29 IF(NF+2)2,2,3000                                         MAIN0450
      30 WRITE OUTPUT TAPE NOUT,14,(AIN(I),I#NI,N2)  MAIN0460
      31 GO TO 90,16,38,50,IC                               MAIN0470
      32 IC#IC+1                                         MAIN0480
      33 FORMAT(I3,6X,5I3,8F6.0)                           MAIN0490
      34 FORMAT(6I3,8E12.5)                                         MAIN0500
      35 FORMAT(IH IIX,5I3,8F11.5)                           MAIN0510
C ***** READ FORMAT 2 TRAILER CARDS *****
      36 NCD#NCD+1                                         MAIN0520
      37 IF(ISAVE)44,40,40                                         MAIN0530
      38 READ INPUT TAPE IN,33,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0540
      39 IF(ISAVE)46,46,42                                         MAIN0550
      40 WRITE OUTPUT TAPE NSR,34,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0560
      41 GO TO 46                                         MAIN0570
      42 READ INPUT TAPE NSR,34,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0580
      43 WRITE OUTPUT TAPE NOUT,35,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0590
      44 GO TO 32                                         MAIN0600
      45 WRITE OUTPUT TAPE NOUT,35,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0610
      46 GO TO 32                                         MAIN0620
      47 WRITE OUTPUT TAPE NOUT,35,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0630
      48 GO TO 32                                         MAIN0640
      49 WRITE OUTPUT TAPE NOUT,35,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)  MAIN0650
      50 GO TO 32                                         MAIN0660

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C ***** READ FORMAT 3 TRAILER CARD *****
50 INN#IN          MAIN0660
IF(ISAVE)52,54,54   MAIN0670
52 INN#NSR         MAIN0680
54 READ INPUT TAPE INN,4,(TITLE2(I),I#1,I2)
WRITE OUTPUT TAPE NOUT,5,(TITLE2(I),I#1,I2)
IF(ISAVE)90,90,56   MAIN0690
56 WRITE OUTPUT TAPE NSR,4,(TITLE2(I),I#1,I2)
C ***** EXECUTE INSTRUCTION *****
90 NJ#NFI/100       MAIN0700
NJ2#NFI-NJ*100     MAIN0710
NJ3#XMODF(NJ2,10)  MAIN0720
IF(NJ-I2)98,92,92   MAIN0730
92 CALL SPARE(NFI)  MAIN0740
IF(NG)94,8,94       MAIN0750
94 CALL ERPNT(0.,NFI)  MAIN0760
GO TO 8             MAIN0770
C *****BRANCH TABLE FOR FUNCTION TYPES*****
98 GO TO (100,200,300,400,500,600,700,800,900,1000,1100),NJ  MAIN0780
C *****STRUCTURE ANALYSIS FUNCTIONS*****
100 GO TO (101,101,104,104,94),NJ2  MAIN0790
101 CALL SEARCH    MAIN0800
GO TO 8             MAIN0810
C ***** ANISOTROPIC TEMP FACTOR OUTPUT *****
104 DO 164 I#1,NATOM  MAIN0820
IF(XMODF(I,14)-1)134,114,134  MAIN0830
114 WRITE OUTPUT TAPE NOUT,6,(TITLE(J),J#1,I2)
WRITE OUTPUT TAPE NOUT,129  MAIN0840
129 FORMAT(IH3DX,4HATOM3X,16HRMS DISPLACEMENT3X,3IHRMS BASEDMAIN0850
  CN REFERENCE17X,29HPROBABILITY COVARIANCE MATRIX)  MAIN0860
134 TI#55501.+FLOAT(I)*100000.  MAIN0870
CALL PAXES(TI,-3)  MAIN0880
IF(NG)144,154,144  MAIN0890
144 CALL ERPNT(TI,104)  MAIN0900
149 FORMAT(IH01DX,A6,F10.6,6X,3F12.7,10X,3F12.7)  MAIN0910
154 WRITE OUTPUT TAPE NOUT,149,CHEM(I),RMS(I),(PAC(J,I),J#1,3),(Q(J,I) MAIN0920
  ,J#1,3)  MAIN0930
164 WRITE OUTPUT TAPE NOUT,159,(RMS(K),(PAC(J,K),J#1,3),(Q(J,K),J#1,3) MAIN0940
  ,K#2,3)  MAIN0950
159 FORMAT(IH 16X,F10.6,6X,3F12.7,10X,3F12.7)  MAIN0960
GO TO 8             MAIN0970
C *****PLOTTER INITIALIZE,FRAME ADVANCE,TERMINATE FUNCTIONS*****MAIN0980
200 CALL F200        MAIN0990
GO TO 8             MAIN1000
300 GO TO (301,302,303,94),NJ2  MAIN1010
C *****PLOT DIMENSIONS*****
301 IF(AIN(1))321,321,311  MAIN1020
311 XLNG(1)#AIN(1)  MAIN1030
321 IF(AIN(2))341,341,331  MAIN1040
331 XLNG(2)#AIN(2)  MAIN1050
341 IF(AIN(3))361,361,351  MAIN1060
351 VIEW#AIN(3)  MAIN1070
361 IF(AIN(4))381,381,371  MAIN1080
371 BRCR#AIN(4)  MAIN1090
381 WRITE OUTPUT TAPE NOUT,389,XLNG(1),XLNG(2),BRDR  MAIN1100
389 FORMAT(IH01DX,1IHPLOT LIMITSF6.2,3H BYF6.2,15H IN. INCLUDINGF6.2,MAIN1110
  112H IN. MARGIN)  MAIN1120
391 WRITE OUTPUT TAPE NOUT,399,VIEW  MAIN1130
399 FORMAT(IH 10X,13HVIEW DISTANCEF7.3,7H INCHES)  MAIN1140
GO TO 8             MAIN1150
C *****LEGEND ROTATION*****
302 THETA#AIN(1)  MAIN1160
TI#THETA*.01745329252  MAIN1170
COSTH#COSF(TI)  MAIN1180
SINTH#SINF(TI)  MAIN1190
DO 312 J#1,9       MAIN1200
312 SYMB(J,I)#0.  MAIN1210
SYMB(I,1)#COSTH  MAIN1220
SYMB(2,2)#COSTH  MAIN1230
SYMB(3,3)#1.  MAIN1240

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SYMB(2,I)#SINTH                                MAINI360
SYMB(1,2)#-SINTH                               MAINI370
WRITE OUTPUT TAPE NOUT,319,THETA                MAINI380
319 FORMAT(IH01DX,44HREGULAR TITLE AND SYMBOL ROTATION IN DEGREESF8.2) MAINI390
GO TO 8                                         MAINI400
C      ***** RETRACE DISPLACEMENT *****
303 DISP#AIN(1)                                 MAINI410
WRITE OUTPUT TAPE NOUT,313,DISP                 MAINI420
313 FORMAT(IH01DX,22HRETRACE DISPLACEMENT #F7.4,5H INCH) MAINI430
GO TO 8                                         MAINI440
C      *****ATOM LIST FUNCTIONS*****
400 GO TO (401,401,401,490,94,94,94,94,94,410,401,401,401,94),NJ2 MAINI450
401 CALL F400                                    MAINI460
GO TO 490                                       MAINI470
410 LATM#0                                     MAINI480
DO 420 I#1,500                                 MAINI490
DO 420 J#1,4                                   MAINI500
420 ATCMS(J,I)#0.                             MAINI510
490 IF(LATM)8,8,491                            MAINI520
491 WRITE OUTPUT TAPE NOUT,499,(ATOMS(I,I),I#1,LATM) MAINI530
499 FORMAT(IH01DX,23HCNTENTS OF ATOMS ARRAY/(15X,10F10.0)) MAINI540
GO TO 8                                         MAINI550
C      *****CARTESIAN COORDINATE SYSTEM FUNCTIONS*****
500 CALL F500                                    MAINI560
IF(NJ3-3)507,539,539                           MAINI570
507 WRITE OUTPUT TAPE NOUT,529                  MAINI580
WRITE OUTPUT TAPE NOUT,519,((REFV(J,I),I#1,3),(AAREV(J,I),I#1,3),JMAINI620
I#1,3)                                         MAINI590
GO TO 8                                         MAINI600
509 FORMAT(IH01DX, 49HORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXEMAINI650
1S18X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VECMAINI660
2TOR8X,8HZ VECTOR)                            MAINI670
519 FORMAT(IH IDX,3E16.7,8X,3E16.7)             MAINI680
529 FORMAT(IH01DX,51HORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXMAINI690
1E16X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HY VECTOR8X,8HY VEMAINI700
2CTOR8X,8HZ VECTOR)                          MAINI710
539 WRITE OUTPUT TAPE NOUT,509                  MAINI720
WRITE OUTPUT TAPE NOUT,519,((WRKV(J,I),I#1,3),(AAWRK(J,I),I#1,3),JMAINI730
I#1,3)                                         MAINI740
GO TO 8                                         MAINI750
C      *****PLOT CENTERING FUNCTIONS*****
600 CALL F600                                    MAINI760
WRITE OUTPUT TAPE NOUT,609,X0(1),X0(2),SCAL1,SCAL2 MAINI770
609 FORMAT(IH01DX,31HORIGIN POINT IN PLOTTER COORD.(F6.2,2H ,F6.2,8H )MAINI790
I IN. / IIX,15HOVERALL SCALE #F6.3,32H INCH/ANGSTROM ELLIPSOID SCAMAINI800
2LE #F6.3)                                     MAINI810
GO TO 391                                       MAINI820
C      *****ELLIPSOID AND SYMBOL PLOT FUNCTIONS*****
C      *****FILL OUT DETAILS FOR SPECIAL MODELS*****
700 GO TO (701,702,704,705,709,94),NJ3        MAINI830
701 AIN(3)#8.                                  MAINI840
GO TO 703                                       MAINI850
702 AIN(3)#0.                                  MAINI860
703 AIN(1)#4.                                  MAINI870
AIN(2)#0.                                      MAINI880
AIN(4)#0.                                      MAINI890
GO TO 709                                       MAINI900
704 AIN(1)#3.                                  MAINI910
AIN(2)#-5.                                     MAINI920
GO TO 706                                       MAINI930
705 AIN(1)#1.                                  MAINI940
AIN(2)#0.                                      MAINI950
706 AIN(3)#1.                                  MAINI960
AIN(4)#5.                                      MAINI970
709 CALL F700                                    MAINI980
GO TO 8                                         MAINI990
C      *****BCND FUNCTIONS*****
800 CALL F800                                    MAIN2000
GO TO 8                                         MAIN2010
C      *****TITLE FUNCTCNS*****

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900 CALL F900          MAIN2060
GO TO 8               MAIN2070
C   *****CELL OUTLINE FUNCTIONS*****
1000 CALL F1000         MAIN2080
GO TO 8               MAIN2090
C   *****SAVE SEQUENCE FUNCTIONS*****
1100 IF(NJ2-2)1101,1102,1103  MAIN2100
1101 ISAVE#1           MAIN2120
GO TO 1104           MAIN2130
1102 ISAVE#0           MAIN2140
J#-1
WRITE OUTPUT TAPE NSR,13,J,NFI,(AIN(I),I#1,7)  MAIN2160
END FILE NSR        MAIN2180
GO TO 1104           MAIN2190
1103 ISAVE#-1         MAIN2200
1104 REWIND NSR       MAIN2210
GO TO 8               MAIN2220
3000 CALL EXIT        MAIN2230
END                  MAIN2240

*LIST8
*LABEL
      FUNCTION ARCCOS(X)          ARCC0010
C     ARCCOS(X) IN DEGREES        ARCC0020
      IF(1.0-ABSF(X))1,2,2       ARCC0030
1 X#SIGNF(1.0,X)           ARCC0040
2 IF(X)3,4,5               ARCC0050
3 ARCCOS#180.0+ATANF(SQRTF(1.0-X*X)/X)*57.29577951  ARCC0060
GO TO 6                  ARCC0070
4 ARCCOS#90.0             ARCC0080
GO TO 6                  ARCC0090
5 ARCCOS#ATANF(SQRTF(1.0-X*X)/X)*57.29577951  ARCC0100
6 RETURN                 ARCC0110
END                      ARCC0120

*LIST8
*LABEL
      SUBROUTINE ATOM(QA,Z)          ATOM0010
C     ATOM COORDINATE SUBROUTINE    ATOM0020
      DIMENSION X(3),Z(3)           ATOM0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)  ATOM0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) ATOM0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) ATOM0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ATOM0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  ATOM0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) ATOM0090
      DIMENSION XLNG(3),X0(3),XT(3)          ATOM0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  ATOM0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ATOM0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1 ATOM0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2  ATOM0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,X0,XT          ATOM0150
      K#QA/100000.0          ATOM0160
      IF(K)109,109,117      ATOM0170
109 X(1)#0.0           ATOM0180
X(2)#0.0           ATOM0190
X(3)#0.0           ATOM0200
GO TO 125           ATOM0210
117 IF(K-NATOM)119,119,503  ATOM0220
503 NG#5           ATOM0230
GO TO 325           ATOM0240
119 D0123J#1,3       ATOM0250
123 X(J)#P(J,K)       ATOM0260
125 TA#ABSF(QA)       ATOM0270
      KSYM#MODF(TA,100000.0)  ATOM0280
      KT#KSYM/100          ATOM0290
      KS#KSYM-100*KT       ATOM0300
      IF(KS-NSYM)203,203,403  ATOM0310
403 NG#4           ATOM0320
GO TO 325           ATOM0330
203 IF(KS)403,205,213  ATOM0340
205 Z(1)#X(1)         ATOM0350

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Z(2)*X(2)                                ATOM0360
Z(3)*X(3)                                ATOM0370
GO TO 311                                 ATOM0380
213 DO 223 K#I,3                          ATOM0390
Z(K)*TS(K,KS)                            ATOM0400
DO 223 J#I,3                          ATOM0410
223 Z(K)*Z(K)+FS(J,K,KS)*X(J)          ATOM0420
311 IF(KT)403,325,313                  ATOM0430
313 IF(KT=555)317,315,317              ATOM0440
315 KSYM#KS                            ATOM0450
GO TO 325                                 ATOM0460
317 K1#KT/100                           ATOM0470
K#KT-100*K1                            ATOM0480
K2#K/10                                ATOM0490
K3#K-10*K2                            ATOM0500
Z(1)*Z(1)+FLOATF(K1-5)                 ATOM0510
Z(2)*Z(2)+FLOATF(K2-5)                 ATOM0520
Z(3)*Z(3)+FLOATF(K3-5)                 ATOM0530
325 RETURN                               ATOM0540
END                                     ATOM0550

*LIST8
*LABEL
      SUBROUTINE AXEQB(AI,X,BI,JJJ)
C      ***** SOLUTION OF MATRIX EQUATION AX#B FOR X *****
C      ***** USES METHOD OF TRIANGULAR ELIMINATION *****
C      ***** B AND X HAVE DIMENSIONS (3,JJJ),A IS ALWAYS (3,3)
C      ***** TO INVERT A MAKE B 3 BY 3 IDENTITY MATRIX *****
C      DIMENSION AI(3,3),A(3,3),B(3,3),BI(3,3),X(3,3)
C      NV#JJJ
C      ***** TRANSFER DATA *****
      DO 2 I#I,3                         AXEQ0010
      DO 2 J#I,3                         AXEQ0020
      IF(NV-J)2,I,1
      1 B(I,J)#BI(I,J)                  AXEQ0030
      2 A(I,J)#AI(I,J)                  AXEQ0040
C      ***** TRIANGULARIZE MATRIX A *****
      DO 17 I#I,2
      S#0.0
      DO 4 J#I,3
      R#ABSF(A(J,I))
      IF(R-S)4,3,3
      3 S#R
      L#J
      4 CCNTINUE
      IF(L-I)5,10,5
      5 DO 6 J#I,3
      S#A(I,J)
      A(I,J)#A(L,J)
      6 A(L,J)#S
      DO 8 J#I,NV
      S#B(I,J)
      B(I,J)#B(L,J)
      8 B(L,J)#S
      10 TEM#A(I,I)
      IF(TEM)11,17,11
      11 IPO#I+1
      DO 16 J#IPO,3
      IF(A(J,I))12,16,12
      12 S#A(J,I)/TEM
      A(J,I)#0.0
      DO 13 K#IPO,3
      13 A(J,K)#A(J,K)-A(I,K)*S
      DO 15 K#I,NV
      15 B(J,K)#B(J,K)-B(I,K)*S
      16 CONTINUE
      17 CONTINUE
C      ***** MODIFY SINGULAR MATRIX *****
      DO 20 I#I,3
      IF(A(I,I))20,19,20
      19 A(I,I)#MAXIF(1.E-25,MAXIF(A(1,1),A(2,2),A(3,3))*1.E-15)

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20 CONTINUE
DO 24 K#I,NV
DO 24 I#I,3
N#4-I
M#N+I
TEM#B(N,K)
IF(3-M)23,21,21
21 DO 22 J#M,3
22 TEM#TEM-A(N,J)*B(J,K)
23 B(N,K)#TEM/A(N,N)
24 X(N,K)#B(N,K)
RETURN
END
AXEQ0490
AXEQ0500
AXEQ0510
AXEQ0520
AXEQ0530
AXEQ0540
AXEQ0550
AXEQ0560
AXEQ0570
AXEQ0580
AXEQ0590
AXEQ0600
AXEQ0610

*LIST8
*LABEL
SUBROUTINE AXES(U,V,X,ITYPE)
C ***** STORE THREE ORTHOGONAL VECTORS EACH 1 ANGSTROM LONG *****
C ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****
C ***** XABSF(ITYPE)#1 W(1)#U,W(2)#(UXV),W(3)#UX(UXV) *****
C ***** XABSF(ITYPE)#2 W(1)#U,W(2)#(UXV)XU,W(3)#(UXV) *****
C ***** ITYPE#0 W(1)#A,W(2)#{AXB}XA,W(3)#{AXB}, ABC#CELL VECTORS ***AXES0010
DIMENSION U(3),V(3),W(3,3),X(3,3)
IT#ITYPE
IF(IT)115,105,115
105 U(1)#1.
U(2)#0.
U(3)#0.
V(1)#0.
V(2)#1.
V(3)#0.
AXES0020
AXES0030
AXES0040
AXES0050
AXES0060
AXES0070
AXES0080
AXES0090
AXES0100
AXES0110
AXES0120
AXES0130
AXES0140
AXES0150
AXES0160
AXES0170
AXES0180
AXES0190
AXES0200
AXES0210
AXES0220
AXES0230
AXES0240
AXES0250
AXES0260
AXES0270
AXES0280
AXES0290
AXES0300
AXES0310

115 DO 125 J#I,3
125 W(J,1)#U(J)
IF(XABSF(IT)-1)145,135,145
135 CALL NORM(U,V,W(1,2),IT)
CALL NORM(U,W(1,2),W(1,3),IT)
GO TO 155
145 CALL NORM(U,V,W(1,3),IT)
CALL NORM(W(1,3),U,W(1,2),IT)
155 DO 195 I#I,3
IF(IT)165,165,175
165 IC#-I
GO TO 195
175 IC#I
195 CALL UNIT(W(I,I),X(I,I),IC)
RETURN
END
AXES010
AXES011
AXES012
AXES013
AXES014
AXES015
AXES016
AXES017
AXES018
AXES019
AXES020
AXES021
AXES022
AXES023
AXES024
AXES025
AXES026
AXES027
AXES028
AXES029
AXES030
AXES031

*LIST8
*LABEL
SUBROUTINE BOND(Z1,Z2,NB)
DIMENSION B(3,3),E(3,3),R(3,3),RT(3,3),S(3,3),U(3,3),VUE(3)
DIMENSION V7(3),W(13,2),X(3),Z(3)
DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)
DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORG(3)
DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
DIMENSION RES(4),RMS(5),SYMR(3,3),TITLE(12),TITLE2(12),TS(3,48)
DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
DIMENSION XLNG(3),XO(3),XT(3)
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORG(3),P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
C ***** OBTAIN POSITIONAL PARAMETERS *****
NG#0
DO 105 J#I,26
105 W(J,1)#0.
W(I,1)#Z1
W(I,2)#Z2
DO 135 I#I,2
BOND0010
BOND0020
BOND0030
BOND0040
BOND0050
BOND0060
BOND0070
BOND0080
BOND0090
BOND0100
BOND0110
BOND0120
BOND0130
BOND0140
BOND0150
BOND0160
BOND0170
BOND0180
BOND0190
BOND0200
BOND0210
BOND0220

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      CALL XYZ(W(1,I),W(4,I),2)          BOND0230
      IF(NG)125,110,125                BOND0240
110 DO 115 J#1,3                  BOND0250
115 W(J+6,I)#XT(J)                BOND0260
      K#W(I,I)/100000.                BOND0270
      L#W(I,I)-FLOAT(K)*100000.       BOND0280
      CALL PLTXY(W(4,I),W(2,I))        BOND0290
      IF(EDGE-BRDR*.25)120,128,128    BOND0300
120 NG#10                         BOND0310
125 NGI#1
      WRITE OUTPUT TAPE NOUT,136,CHEM(K),K,L,(W(J,I),J#2,9) BOND0320
      CALL ERPNT(W(I,I),800)           BOND0330
      GO TO 135                      BOND0340
128 IF(NJ2-ID)130,135,135          BOND0350
130 WRITE OUTPUT TAPE NOUT,136,CHEM(K),K,L,(W(J,I),J#2,9) BOND0360
135 CONTINUE                      BOND0370
136 FORMAT(IH I0X,A6,3H  (I3,IH,I5,4H)  2F8.2,5X,3F8.3,I3X,3F8.4) BOND0380
      IF(NGI)999,140,999              BOND0390
140 CALL DIFV(W(7,1),W(7,2),V7)     BOND0400
      DIST#SQRT(VMV(V7,AA,V7))       BOND0410
      IF(XMODF(NJ2,10)-3)143,142,142 BOND0420
142 HGT#SCALI*.12                 BOND0430
      CALL SIMBOL(W(2,1),W(3,1),HGT,XMODF(XFIXF(W(I,I)/100000.),10),0.,- BOND0440
11)
      CALL SIMBOL(W(2,2),W(3,2),HGT,XMODF(XFIXF(W(I,2)/100000.),10),0.,- BOND0450
12)
      GO TO 570                      BOND0460
143 KODE#KD(5,NB)                 BOND0470
      IF(KODE)145,144,146              BOND0480
144 NBND#0                         BOND0490
      GO TO 148                      BOND0500
145 KODE#-KCDE                    BOND0510
146 NBND#128/2**KODE              BOND0520
C      ***** FIND UPPERMOST ATOM PUT IN POSITION ONE *****
148 IF(VIEW)152,150,152            BOND0530
150 W(I2,1)#1.
      W(I2,2)#1.
      IF(W(6,1)-W(6,2))165,175,175 BOND0540
C      *****VECTOR FROM ATOM TO VIEWPOINT *****
152 DO 160 I#1,2                  BOND0550
      DO 155 J#10,12                BOND0560
155 W(J,I)#-W(J-6,I)              BOND0570
      W(I2,I)#W(I2,I)+VIEW         BOND0580
C      ***** DISTANCE SQUARED TO VIEWPOINT *****
160 W(I3,I)#VV(W(10,I),W(10,I))  BOND0590
      IF(W(13,2)-W(13,1))165,175,175 BOND0600
C      ***** SWITCH ATOMS *****
165 DO 170 J#1,13                BOND0610
      TI#W(J,1)                     BOND0620
      W(J,1)#W(J,2)                 BOND0630
170 W(J,2)#TI                     BOND0640
C      ***** FORM IDEMFACTOR MATRIX *****
175 DO 180 J#1,3                  BOND0650
      E(J,J)#1.
      E(J+1,I)#0.
180 E(J+5,I)#0.                   BOND0660
C      ***** FORM VECTOR SET RADIAL TO BOND *****
      CALL DIFV(W(4,2),W(4,1),DA(I,3)) BOND0670
      CALL UNIT(DA(I,3),V3,I)         BOND0680
      T6#ABSF(V3(I))
      IF(.9994-T6)390,185,185       BOND0690
185 TI#CD(3,NB)/SCAL2             BOND0700
      CALL AXES(V3,E(I,3),B,I)        BOND0710
      DO 190 J#1,3                  BOND0720
      DA(J,1)#-B(J,2)*TI             BOND0730
190 DA(J,2)#-B(J,3)*TI             BOND0740
      IF(NBND)500,500,195             BOND0750
195 CALL RADICAL(3)                BOND0760
C      ***** DERIVE QUADRICS FOR EACH ATOM *****
      DO 380 III#1,2                 BOND0770

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        CALL PAXES(W(I,II),2)                                BOND0930
        IF(NG)205,210,205
205  CALL ERPNT(W(I,II),800)
        GO TO 999
C      ***** DCES BOND GO TO ELLIPSOID OR TO ENVELOPE *****
210  TI#3-II*2                                         BOND0940
        DO 212 J#I,3
        V3(J)#V3(J)*TI                                     BOND0950
212  VUE(J)#0.                                         BOND0960
        IF(KD(5,NB))260,260,215
215  CALL UNIT(W(I0,II),R(I,3),I)                      BOND0970
        IF(VMV(V3,Q,R(I,3)))220,260,260
C      ***** ESTABLISH VIEW COORDINATE SYSTEM *****
220  IBND#0                                         BOND0980
        IF(VIEW)225,225,230
C      ***** DERIVE TANGENT CYLINDER *****
225  CCNE#0.                                         BOND0990
        GO TO 240
C      ***** DERIVE TANGENT CONE *****
230  CONE#SCL*SCL/W(I3,II)                            BOND1000
        CALL NORM(E(I,2),R(I,3),R(I,I),I)                 BOND1010
        CALL UNIT(R(I,I),R(I,I),I)                         BOND1020
        CALL NORM(R(I,3),R(I,I),R(I,2),I)                 BOND1030
        DO 235 I#I,3
        DO 235 J#I,3
235  RT(I,J)#R(J,I)                                    BOND1040
C      ***** BASE ELLIPSOID ON VIEW COORDINATE SYSTEM *****
        CALL MM(RT,Q,U)
        CALL MM(U,R,Q)
240  TI#I./(CONE-Q(3,3))                            BOND1050
        T2#CONE*TI                                       BOND1060
        DO 250 J#I,2
        DO 245 K#I,2
245  S(K,J)#Q(K,J)+Q(K,3)*Q(J,3)*TI               BOND1070
        S(3,J)#Q(3,J)*T2                               BOND1080
250  S(J,3)#Q(J,3)*T2                               BOND1090
        S(3,3)#Q(3,3)*T2                               BOND1100
        IF(CONE)252,270,252
252  DO 255 J#I,3
255  VUE(J)#-W(J+9,II)/SCL                          BOND1110
C      ***** BASE TANGENT CONE ON WORKING SYSTEM *****
        CALL MM(R,S,U)
        CALL MM(U,RT,S)
        TS#0.
        GO TO 300
C      ***** TRANSFER ELLIPSOID *****
260  DO 265 J#I,9
265  S(J,I)#Q(J,I)
        IBND#II
270  TS#I.
C      ***** CHECK FOR BCND TAPER *****
300  IF(II-2)305,310,310
305  RADIUS#I.+T6*TAPER
        GO TO 320
310  RADIUS#I.-T6*TAPER
320  CALL MV(S,V3,V4)
        T2#VV(V3,V4)
C      ***** COMPUTE BOND INTERSECTION *****
        KL#5-II-II
        DO 360 K#I,65,4
        DO 325 J#I,3
        V6(J)#D(J,K)*RADIUS
325  V5(J)#V6(J)+VUE(J)
        T3#VV(V5,V4)
        T4#T3-T2*(VMV(V5,S,V5)-T5)
        IF(T4)330,335,335
330  NG#13
        CALL ERPNT(W(I,II),800)
        GO TO 999
335  T4#SQRTF(T4)

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T1#(T4-T3)/T2                                BOND1630
T3#(-T4-T3)/T2                               BOND1640
L#K+KL-1                                     BOND1650
DO 360 J#1,3                                 BOND1660
D(J,L)#{V6(J)+T1*V3(J))*SCL                BOND1670
360 D(J,L+1)#{-V6(J)-T3*V3(J))*SCL        BOND1680
CALL PROJ(D(I,KL),DP(I,II),W(4,II),X0,VIEW,I,65,4) BOND1690
IF(IBND-I)370,365,370                         BOND1700
365 CALL PROJ(D(I,KL+5),DP(I,II+68),W(4,II),X0,VIEW,I,61,4) BOND1710
GO TO 380                                     BOND1720
C      **** RETRACE TOP HALF *****
370 DO 375 K#4,64,4                           BOND1730
L#K+II                                       BOND1740
M#L+64                                       BOND1750
N#66-L                                       BOND1760
DP(I,M)#DP(I,N)                            BOND1770
375 DP(2,M)#DP(2,N)                          BOND1780
380 CONTINUE                                    BOND1790
C      **** CHECK FOR OVERLAP OR HIDDEN BOND *****
DO 395 K#1,65,32                            BOND1800
T1#0.                                         BOND1810
T2#0.                                         BOND1820
DO 385 J#1,2                                 BOND1830
T1#T1+(DP(J,K)-W(J+1,I))**2                BOND1840
385 T2#T2+(DP(J,K+1)-W(J+1,I))**2        BOND1850
IF(T2-T1)390,390,395                         BOND1860
390 NG#14                                     BOND1870
CALL ERPNT(W(I,2),800)                      BOND1880
GO TO 999                                     BOND1890
395 CCNTINUE                                  BOND1900
C      **** DRAW BOND OUTLINE *****
CALL DRAW(DP(I,I),0.,0.,3)                  BOND1910
DO 415 K#5,129,4                           BOND1920
415 CALL DRAW(DP(I,K),0.,0.,2)                BOND1930
DO 420 K#2,66,4                           BOND1940
420 CALL DRAW(DP(I,K),0.,0.,2)                BOND1950
CALL DRAW(DP(I,65),0.,0.,2)                  BOND1960
C      **** DRAW BOND DETAIL *****
425 K#65                                     BOND1970
430 K#K-NBND                                 BOND1980
IF(K-I)500,500,435                         BOND1990
435 CALL DRAW(DP(I,K),0.,0.,3)                BOND2000
CALL DRAW(DP(I,K+1),0.,0.,2)                 BOND2010
K#K-NBND                                   BOND2020
IF(K-I)500,500,440                         BOND2030
440 CALL DRAW(DP(I,K+1),0.,0.,3)                BOND2040
CALL DRAW(DP(I,K),0.,0.,2)                  BOND2050
GO TO 430                                     BOND2060
500 HGT#CD(4,NB)                            BOND2070
OFF#CD(5,NB)                                BOND2080
IF(HGT)510,570,510                         BOND2090
C      **** PERSPECTIVE BOND LABEL ROUTINE *****
C      **** BASE DECISIONS ON REFERENCE SYSTEM *****
510 K#0                                      BOND2100
CALL DIFV(W(7,2),W(7,1),V7)                  BOND2110
CALL VM(V7,AAREV,V1)                        BOND2120
CALL AXES(V1,E(I,3),U,I)                    BOND2130
DO 535 I#1,3                                 BOND2140
T1#I.                                       BOND2150
IF(I-2)515,515,520                         BOND2160
515 IF(VV(U(I,I),SYMB(I,I)))525,530,530   BOND2170
520 IF(XMODF(I,K,2))530,525,530           BOND2180
525 T1#-I.                                  BOND2190
K#K+1                                     BOND2200
530 DO 535 J#1,3                           BOND2210
U(J,I)#U(J,I)*T1                         BOND2220
535 VT(J,I)#B(J,I)*T1                     BOND2230
DO 540 J#1,3                           BOND2240
540 VT(J,4)#+.5*(W(J+3,I)+W(J+3,2))    BOND2250
C      **** CHECK FOR EXCESS FORESHORTENING *****

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      IF(FORE-ABSF(U(3,1)))545,550,550          BOND2320
545 CALL NORM(U(1,2),SYMB(1,3),VT(1,1),1)      BOND2330
      VT(1,3)#SYMB(1,3)                          BOND2340
      VT(2,3)#SYMB(2,3)                          BOND2350
      VT(3,3)#SYMB(3,3)                          BOND2360
      HGT#CD(6,NB)                                BOND2370
      OFF#CD(7,NB)                                BOND2380
      IF(HGT)550,999,550                          BOND2390
550 TI#CD(8,NB)                                BOND2400
      Z(1)#VT(1,4)-HGT*(23.-3.*TI)/7.           BOND2410
      Z(2)#VT(2,4)+OFF-HGT*.5                   BOND2420
      Z(3)#VT(3,4)                                BOND2430
      ITILT#1                                    BOND2440
      IF(TI)555,560,565                          BOND2450
555 CALL NUMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.1)    BOND2460
      GO TO 570                                  BOND2470
560 CALL NUMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.2)    BOND2480
      GO TO 570                                  BOND2490
565 CALL NUMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.3)    BOND2500
570 ITILT#0                                    BOND2510
      IF(NJ2-I0)580,999,999                      BOND2520
580 WRITE OUTPUT TAPE NOUT,571,DIST            BOND2530
571 FORMAT(IH 59X,I0HDISTANCE #F8.3/IH )       BOND2540
999 RETURN                                     BOND2550
      END                                         BOND2560

*LIST8
*LABEL
      SUBROUTINE DIFV(X,Y,Z)                      DIFV0010
C      VECTOR - VECTOR                           DIFV0020
C      Z(3)#X(3)-Y(3)                          DIFV0030
      DIMENSION X(3),Y(3),Z(3)                  DIFV0040
      DO111I#1,3                                DIFV0050
111 Z(I)#X(I)-Y(I)                          DIFV0060
      RETURN                                     DIFV0070
      END                                         DIFV0080

*LIST8
*LABEL
      SUBROUTINE DRAW(W,DX,DY,NPEN)              DRAW0010
      DIMENSION W(3),X(3),Y(3),Z(3)            DRAW0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) DRAW0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) DRAW0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) DRAW0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) DRAW0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  DRAW0070
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) DRAW0080
      DIMENSION XLNG(3),XO(3),XT(3)             DRAW0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D DRAW0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD DRAW0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI DRAW0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 DRAW0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT        DRAW0140
      Y(1)#W(1)+DX                            DRAW0150
      Y(2)#W(2)+DY                            DRAW0160
      IF(ITILT)115,140,115                      DRAW0170
C      ***** RCTATE FOR PERSPECTIVE TITLE *****
115 Y(3)#W(3)                                DRAW0180
      DO120 I#1,3                                DRAW0200
120 Z(I)#Y(I)-VT(I,4)                          DRAW0210
      DO130 I#1,3                                DRAW0220
130 X(I)#VT(I,1)*Z(I)+VT(I,2)*Z(2)+VT(I,3)*Z(3)+VT(I,4)        DRAW0230
      CALL PLTXY(X,Y)                          DRAW0240
C      ***** CHECK BOUNDARY *****
140 DO160 J#1,2                                DRAW0260
      IF(Y(J)-XLNG(J)+.1)150,150,145          DRAW0270
145 Y(J)#XLNG(J)-.1                          DRAW0280
150 IF(Y(J)-.1)155,160,160                    DRAW0290
155 Y(J).1                                     DRAW0300
160 CCNTINUE                                 DRAW0310
      CALL PLCT(Y(1),Y(2),NPEN)                 DRAW0320
      RETURN                                     DRAW0330

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END                                DRAW0340
*LISTB
*LABEL
      SUBROUTINE EIGEN (W,VALU,VECT)
C      ***** EIGENVALUES AND EIGENVECTORS OF 3X3 MATRIX *****
C      DIMENSION W(3,3),VALU(3),VECT(3,3),A(3,3),B(3,3),V(3),U(3)
C      COMMON NG
C      ***** STATEMENT FUNCTION *****
C      PHIF(Z)#{(B2-Z)*Z+B1)*Z+B0
C      ***** START OF PROGRAM *****
C      ERRND#5.E-8
C      SIGMA#0.
      DO 115 J#1,3
      DO 115 I#1,3
      TEM#W(I,J)
      A(I,J)#TEM
115  SIGMA#SIGMA+TEM*TEM
C      ***** CHECK FOR NULL MATRIX *****
      IF(SIGMA)230,230,120
120  SIGMA#SQRTF(SIGMA)
C      ***** FORM CHARACTERISTIC EQUATION *****
      B2#A(1,1)+A(2,2)+A(3,3)
      B1#-A(1,1)*A(2,2)-A(1,1)*A(3,3)-A(2,2)*A(3,3)+A(1,3)*A(3,1)
      I+A(2,3)*A(3,2)+A(1,2)*A(2,1)
      B0#A(1,1)*A(2,2)*A(3,3)+A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(3,2)*A(2,1)-EIGE0220
      I(A(1,3)*A(3,1)*A(2,2)-A(1,1)*A(2,3)*A(3,2)-A(1,2)*A(2,1)*A(3,3)
C      ***** FIRST ROOT BY BISECTION *****
      X#0.
      Y#SIGMA
      TEM#PHIF(SIGMA)
      VNEW#0.0
      IF(B0)135,250,145
135  IF(TEM)140,140,165
140  Y#-Y
      GO TO 165
145  Y#0.
      X#SIGMA
      IF(TEM)165,165,150
150  X#-X
C      ***** NOW PHIF(X).LT.0.AND.PHIF(Y).GT.0. *****
165  VNEW#(X+Y)*.5
      DO 225 I#1,40
175  IF(PHIF(VNEW))180,250,185
180  X#VNEW
      GO TO 200
185  Y#VNEW
200  VOLD#VNEW
      VNEW#(X+Y)*.5
      TEM#ABSF(VOLD-VNEW)
      IF(ITEM-ERRND)250,250,205
205  IF(VOLD)210,225,210
210  IF(ABSF(ITEM/VOLD)-ERRND)250,250,225
225  CONTINUE
C      ***** DID NOT CONVERGE, SET ERROR INDICATOR *****
230  NG#6
      GO TO 400
C      ***** STORE FIRST ROOT *****
250  U(3)#VNEW
C      ***** DEFLATE *****
      C1#B2-VNEW
      C0#B1+C1*VNEW
C      ***** SOLVE QUADRATIC *****
      TEM#C1*C1+4.*C0
      IF(ITEM)255,265,260
C      ***** IGNORE IMAGINARY COMPONENT OF COMPLEX ROOT *****
255  TEM#0.
      GO TO 265
260  TEM#SQRTF(TEM)
265  U(1)#.5*(C1-TEM)
      U(2)#.5*(C1+TEM)

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C      ***** SORT ROOTS *****
DO 275 J#I,2
IF(U(J)-U(3))275,275,270
270 TEM#U(J)
U(J)#U(3)
U(3)#TEM
275 CCNTINUE
LLL#-2
DO 375 III#I,2
C      ***** CHECK FOR MULTIPLE ROOTS *****
TEM#ERRND*100.
NG#0
L#I
DO 305 I#I,2
IF(U(I+1)-U(I)-TEM)300,300,290
290 IF(U(I))295,305,295
295 IF(ABSF((U(I+1)-U(I))/U(I))-TEM)300,300,305
300 L#L-I
NG#NG-2*I
305 CCNTINUE
IF(LLL-L)308,400,400
308 LLL#L
C      ***** EIGENVECTOR ROUTINE *****
DO 375 III#I,3
TI#U(11)
IF(L)315,310,322
C      ***** TWO VECTORS NULL FOR DOUBLE ROOT *****
310 IF(NG+5-III)315,322,315
C      ***** ALL VECTORS NULL FOR TRIPLE ROOT *****
315 DO 320 J#I,3
320 VECT(J,II)#0.0
GO TO 375
322 DO 325 J#I,3
325 A(J,J)#W(J,J)-TI
SMAX#0.0
DO 355 I#I,3
II#I
IF(I-2)335,335,340
335 II#I+
340 B(I,I)*A(I,2)*A(II,3)-A(I,3)*A(II,2)
B(I,2)*A(I,3)*A(II,1)-A(I,1)*A(II,3)
B(I,3)*A(I,1)*A(II,2)-A(I,2)*A(II,1)
TEM#B(I,1)**2+B(I,2)**2+B(I,3)**2
IF(TEM-SMAX)355,355,350
350 SMAX#TEM
IMAX#I
355 CCNTINUE
IF(SMAX)353,353,360
353 NG#7
GO TO 375
360 SMAX#SORTF(SMAX)
DO 365 J#I,3
365 V(J)#B(IMAX,J)/SMAX
C      ***** REFIN EIGENVECTOR *****
CALL AXEQB(A,V,V,I)
TEM#MAX1(ABSF(V(1)),ABSF(V(2)),ABSF(V(3)))
DO 370 J#I,3
370 V(J)#V(J)/TEM
CALL UNIT(V,VECT(I,II),I)
C      ***** REFIN EIGENVALUE *****
TI#VMV(VECT(I,II),W,VECT(I,II))
U(II)#TI
375 VALU(II)#TI
400 RETURN
END
*LIST8
*LABEL
      SUBROUTINE ERPNT(T1,N)                                ERPN0010
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)   ERPN0020
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)ERPN0030

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DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3)  ERPN0040
DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  ERPN0050
DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)    ERPN0060
DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)  ERPN0070
DIMENSION XLNG(31),XO(3),XT(3)                                     ERPN0080
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  ERPN0090
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD  ERPN0100
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI  ERPN0110
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2  ERPN0120
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ERPN0130
WRITE OUTPUT TAPE NOUT,I15,NG,TI,N                                 ERPN0140
115 FORMAT(IH 10X,I0HFAULT NG #I3,F10.0,I6/IH )
NG#0
RETURN
END
*LIST8
*LABEL
      SUBROUTINE F200
      DIMENSION PLA(2000)                                         F2000010
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F2000020
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F2000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F2000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F2000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F2000070
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F2000080
      DIMENSION XLNG(31),XO(3),XT(3)                               F2000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D F2000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F2000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI F2000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2  F2000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                            F2000140
C      ***** CALCOMP CONTROL *****
C      IF(NJ2-1)216,210,212                                         F2000150
C      210 CALL PLCTS(PLA(2000),1998,LTNO)                         F2000160
C      ***** FCR CDC 1604 A USE 210 CALL PLOTS(PLA,2000,LTNO) ***** F2000175
C      ***** FCR IBM 7090 USE 210 CALL PLOTS(PLA(2000),1998,LTNO) ***** F2000176
C      GO TO 216
C      212 CALL PLCT(AIN(1),AIN(2),-3)                             F2000190
C      216 RETURN
C      END
*LIST8
*LABEL
      SUBROUTINE F400
      ***** ATOM LIST FUNCTIONS *****
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F4000010
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F4000020
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F4000040
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F4000050
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F4000060
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F4000070
      DIMENSION XLNG(31),XO(3),XT(3)                               F4000080
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D F4000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F4000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI F4000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2  F4000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                            F4000140
      NG#0
      IF(LATM)402,402,400                                         F4000150
400 DO 401 I#1,LATM                                           F4000170
401 CALL ATOM(ATOMS(1,I),ATOMS(2,I))                           F4000180
402 IF(XMODF(NJ2,I)-1)499,404,403                           F4000190
403 CALL SEARCH
GO TO 499
C      ***** STORES (401) OR REMOVES (411) RUNS OF ATOMS *****
C      ***** RUN HIERARCHY # ATOM NO./SYM/ A/B/C TRANS. *****
404 I#1
C      ***** FIND RUNS IN AIN ARRAY *****
405 TI#AIN(I)
IF(TI)410,410,420
410 II#II+1

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        IF(140-II)499,405,405          F4000290
420  JJ#II                         F4000300
C   ***** SET INITIAL RUN VALUES *****
M1#TI/100000.                      F4000310
M2#MODF(TI,100.)                   F4000320
M5#MODF(TI/100.,1000.)              F4000330
IF(M5)422,422,423                  F4000340
F4000350
422  M5#555                         F4000360
423  M3#M5/100                      F4000370
M4#XMODF(M5/10,10)                 F4000380
M5#XMODF(M5,10)                   F4000390
425  JJ#JJ+1                        F4000400
IF(140-JJ)435,430,430              F4000410
430  T2#-AIN(JJ)                   F4000420
IF(T2)435,425,440                  F4000430
435  II#JJ-1                       F4000440
C   ***** SET TERMINAL VALUES FOR DEGENERATE RUN *****
NI#MI                           F4000450
N2#M2                           F4000460
N3#M3                           F4000470
N4#M4                           F4000480
N5#M5                           F4000490
GO TO 450                        F4000500
F4000510
440  II#JJ                         F4000520
C   ***** SET TERMINAL RUN VALUES *****
NI#T2/100000.                     F4000530
N2#MODF(T2,100.)                 F4000540
N5#MODF(T2/100.,1000.)            F4000550
F4000560
IF(N5)445,445,446                  F4000570
F4000580
445  N5#555                         F4000590
446  N3#N5/100                      F4000600
M4#XMODF(N5/10,10)                F4000610
M5#XMODF(N5,10)                  F4000620
C   ***** LCOP THROUGH ALL RUNS *****
450  DO 490  L5#M5,N5               F4000630
DO 490  L4#M4,N4                  F4000640
DO 490  L3#M3,N3                  F4000650
DO 490  L2#M2,N2                  F4000660
DO 490  LI#MI,N1                  F4000670
VI(1)#FLOATF(L1)*100000.+FLOATF(L3*10000+L4*1000+L5*100+L2) F4000680
CALL ATOM(VI(1),VI(2))           F4000690
IF(NG)455,458,455                  F4000700
455  CALL ERPNT(VI(1),401)         F4000710
GO TO 490                          F4000720
458  CALL STORE                    F4000730
490  CONTINUE                      F4000740
GO TO 410                          F4000750
499  RETURN                         F4000760
END                               F4000770

*LIST8
*LABEL
      SUBROUTINE F500                F5000010
      DIMENSION RM(3,3),V(3,4)         F5000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F5000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) F5000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F5000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F5000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) F5000070
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F5000080
      DIMENSION XLNG(3),XO(3),XT(3)    F5000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D F5000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F5000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI F5000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 F5000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT F5000140
      NG#
      IF(NJ2-I)599,501,510             F5000150
501  TI#AIN(I)                     F5000160
      CALL ATOM(TI,ORGN)               F5000170
      IF(NG)502,504,502                  F5000180
                                         F5000190

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502 CALL ERPNT(TI,501) F5000200
CALL EXIT F5000210
504 DO 506 K#1,4 F5000220
   T1#AIN(K+1) F5000230
   CALL ATCM(TI,V(I,K)) F5000240
   IF(NG)502,506,532 F5000250
506 CONTINUE F5000260
   DO 507 J#1,3 F5000270
     V1(J)#V(J,2)-V(J,1) F5000280
507 V2(J)#V(J,4)-V(J,3) F5000290
   IND#-1 F5000300
   IF(AIN(7))509,509,508 F5000310
508 IND#-2 F5000320
509 CALL AXES(V1,V2,REFV,IND) F5000330
   GO TO 562 F5000340
510 DO 552 L#1,139,2 F5000350
   I#AIN(L) F5000360
   IF(I)532,552,512 F5000370
512 X#AIN(L+1)*0.31745329252 F5000380
   TI#COSF(X) F5000390
   T2#SINF(X) F5000400
   I3#XMODF(I+2,3)+1 F5000410
   I1#XMODF(I3,3)+1 F5000420
   I2#XMODF(I1,3)+1 F5000430
   RM(I1,I1)#TI F5000440
   RM(I1,I2)#T2 F5000450
   RM(I1,I3)#0.0 F5000460
   RM(I2,I1)#-T2 F5000470
   RM(I2,I2)#TI F5000480
   RM(I2,I3)#0.0 F5000490
   RM(I3,I1)#0.0 F5000500
   RM(I3,I2)#0.0 F5000510
   RM(I3,I3)#1.0 F5000520
   CALL MM(REFV,RM,V) F5000530
   IF(NJ2-3)518,525,599 F5000540
518 DO 522 J#1,9 F5000550
522 REFV(J,1)#V(J,1) F5000560
   GO TO 552 F5000570
525 DO 528 J#1,9 F5000580
528 WRKV(J,1)#V(J,1) F5000590
   GO TO 552 F5000600
532 IF(NJ2-3)535,552,599 F5000610
535 I#XMODF(-1,3) F5000620
   DO 542 J#1,I F5000630
   DO 542 K#1,3 F5000640
   TI#REFV(K,3) F5000650
   REFV(K,3)*REFV(K,2) F5000660
   REFV(K,2)*REFV(K,1) F5000670
542 REFV(K,1)#TI F5000680
552 CONTINUE F5000690
   IF(NJ2-3)562,582,599 F5000700
562 CALL MM(AA,REFV,AAREV) F5000710
   DO 572 J#1,9 F5000720
   WRKV(J,1)#REFV(J,1) F5000730
572 AAWRK(J,1)#AAREV(J,1) F5000740
   GO TO 599 F5000750
582 CALL MM(AA,WRKV,AAWRK) F5000760
599 RETURN F5000770
END F5000780

*LIST8
*LABEL
      SUBROUTINE F600 F6000010
C      ***** SCALING AND CENTERING FUNCTIONS *****
      DIMENSION MAX(3),SCAL(4),X(3),XMAX(3),XMIN(3),Z(2) F6000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F6000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) F6000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F6000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F6000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) F6000070
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F6000080
                                          F6000090

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DIMENSION XLNG(3),XO(3),XT(3) F6000100
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D F6000110
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LAT*,LTNO,NATOM,NCD F6000120
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI F6000130
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 F6000140
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT F6000150
C **** DEL # I. FOR INCRUMENTING FUNCTIONS **** F6000160
C **** DEL # O. FOR REGULAR FUNCTIONS **** F6000170
DEL#FLOAT(XMODF(NJ2/I0,2)) F6000180
NJ2#XMODF(NJ2,I0) F6000190
C ***** EXPLICIT ORIGIN AND SCALE ***** F6000200
IF(AIN(1))602,604,602 F6000210
602 XO(1)#AIN(1)+XO(1)*DEL F6000220
604 IF(AIN(2))606,608,606 F6000230
606 XO(2)#AIN(2)+XO(2)*DEL F6000240
608 IF(AIN(3))612,612,609 F6000250
609 IF(DEL)611,611,610 F6000260
610 SCAL1#SCAL1*AIN(3) F6000270
GO TO 612 F6000280
611 SCAL1#AIN(3) F6000290
612 IF(AIN(4))616,616,614 F6000300
C ***** SET ELLIPSOID SCALE FACTOR ***** F6000310
614 SCAL2#AIN(4) F6000320
C ***** AUTOMATIC ORIGIN AND/OR SCALE ***** F6000330
616 IF(NJ2-2)790,622,620 F6000340
620 XO(1)#XLNG(1)*.5 F6000350
XO(2)#XLNG(2)*.5 F6000360
622 IF(NJ2-3)625,643,625 F6000370
625 SCAL1#I. F6000380
630 IF(LATM-1)635,635,640 F6000390
635 NG#12 F6000400
CALL ERPNT(0.,602) F6000410
CALL EXIT F6000420
640 DO 650 J#1,3 F6000430
XMAX(J)#-1.E5 F6000440
650 XMIN(J)#1.E5 F6000450
C ***** FIT BOX AROUND SET OF ATOMS ***** F6000460
DO 670 I#1,LATM F6000470
CALL XYZ(ATOMS(I,1),ATOMS(2,I),3) F6000480
IF(NG)652,653,652 F6000490
652 CALL ERPNT(ATOMS(I,1),600) F6000500
GO TO 670 F6000510
653 DO 668 J#1,3 F6000520
T1#ATOMS(J+1,1) F6000530
IF(XMAX(J)-T1)655,660,660 F6000540
655 XMAX(J)#T1 F6000550
MAX(J)#I F6000560
660 IF(T1-XMIN(J))665,668,668 F6000570
665 XMIN(J)#T1 F6000580
668 CCNTINUE F6000590
670 CCNTINUE F6000600
C ***** KM#TOP ATOM ***** F6000610
KM#MAX(3) F6000620
SMULT#I. F6000630
DO 780 M#1,5 F6000640
IF(M-2)740,675,678 F6000650
C ***** CHECK VIEW DISTANCE ***** F6000660
675 IF(VIEW)785,785,680 F6000670
678 IF(NJ2-3)680,785,680 F6000680
680 T1#ATOMS(4,KM)*SMULT F6000690
IF(VIEW*.5-T1)685,690,690 F6000700
C ***** INCREASE VIEW DISTANCE ***** F6000710
685 VIEW#2.*T1 F6000720
C ***** FIND PERSPECTIVE PROJECTION LIMITS ***** F6000730
690 DO 700 J#1,2 F6000740
XMAX(J)#-1.E5 F6000750
700 XMIN(J)#1.E5 F6000760
DO 725 I#1,LATM F6000770
DO 705 J#1,3 F6000780
705 X(J)#ATOMS(J+1,1)*SMULT F6000790

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T2#VIEW/(VIEW-X(3)) F6000800
DO 725 J#1,2 F6000810
TI#X(J)#T2 F6000820
IF(XMAX(J)-TI)710,715,715 F6000830
710 XMAX(J)#TI F6000840
715 IF(TI-XMIN(J))720,725,725 F6000850
720 XMIN(J)#TI F6000860
725 CCNTINUE F6000870
C **** REFINE PARAMETERS **** F6000880
740 IF(NJ2 -3)745,742,755 F6000890
742 SMUL2#1. F6000900
GO TO 765 F6000910
C **** AUTOMATIC SCALE ONLY **** F6000920
745 DO 750 J#1,2 F6000930
T2#X0(J) F6000940
SCAL(J)#{BRDR-T2}/XMIN(J) F6000950
750 SCAL(J+2)#{XLNG(J)-BRDR-T2}/XMAX(J) F6000960
SMUL2#MIN(IF(SCAL(1),SCAL(2),SCAL(3),SCAL(4))) F6000970
GO TO 780 F6000980
C **** AUTOMATIC SCALE AND POSITION **** F6000990
755 DO 760 J#1,2 F6001000
760 SCAL(J)#{(XLNG(J)-BRDR*2.)/(XMAX(J)-XMIN(J))} F6001010
SMUL2#MIN(IF(SCAL(1),SCAL(2))) F6001020
C **** AUTOMATIC POSITION **** F6001030
765 DO 770 J#1,2 F6001040
770 X0(J)#+.5*(XLNG(J)-SMUL2*(XMAX(J)+XMIN(J))) F6001050
780 SMULT#SMULT*SMUL2 F6001060
VIEW#VIEW*SMUL2 F6001070
785 SCAL1#SCAL1*SMULT F6001080
790 SCL#SCAL1*SCAL2 F6001090
RETURN F6001100
END F6001110
*LIST8
*LABEL
SUBROUTINE F700 F7000010
C **** SUBROUTINE TO DRAW ELLIPSOIDS **** F7000020
DIMENSION EYE(3),VIEWV(3),X(3),Z(3) F7000030
DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F7000040
DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) F7000050
DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F7000060
DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F7000070
DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) F7000080
DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F7000090
DIMENSION XLNG(3),X0(3),XT(3) F7000100
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D F7000110
COMMON CA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F7000120
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1 F7000130
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 F7000140
COMMON V3,V4,V5,V6,WRKV,XLNG,X0,XT F7000150
C **** SET ELLIPSOID GRAPHIC DETAILS **** F7000160
ITILT#0 F7000170
NG#0 F7000180
NFIRST#1 F7000190
NPLANE#AIN(1) F7000200
IF(NPLANE-1)720,715,720 F7000210
715 NFIRST#4 F7000220
NPLANE#4 F7000230
720 NSOLID#AIN(2) F7000240
NDCT#64/2**((XABS(F(NSOLID))) F7000250
LINES#AIN(3) F7000260
NDASH#AIN(4) F7000270
CHSYM#AIN(5) F7000280
DH#AIN(6)-CHSYM=17./7. F7000290
DV#AIN(7)-CHSYM=.5 F7000300
C **** ESTABLISH REFERENCE POINT OF VIEW **** F7000310
TI#1.E6 F7000320
IF(VIEW)740,740,735 F7000330
735 TI#VIEW/SCAL1 F7000340
740 DO 745 J#1,3 F7000350
745 EYE(J)#REFV(J,3)*TI+ORGN(J) F7000360

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LNS#-1 F7000370
C ***** LCOP THROUGH ATOM LIST *****
DO 1105 ITOM#1,LATM F7000380
TI#ATOMS(1,ITOM) F7000390
CALL XYZ(TI,X,2) F7000400
IF(NG)758,746,758 F7000410
F7000420
746 CALL PLTXY(X,Z) F7000430
K#TI/100000. F7000440
L#TI-FLOATF(K)*100000. F7000450
IF(NJ2-I0)747,754,754 F7000460
747 LNS#XMODF(LNS+1,18) F7000470
IF(LNS)749,748,749 F7000480
748 WRITE OUTPUT TAPE NOUT,751,(TITLE(I),I#1,12) F7000490
WRITE OUTPUT TAPE NOUT,752 F7000500
749 WRITE OUTPUT TAPE NOUT,750,CHEM(K),K,L,Z(1),Z(2),(X(I),I#1,3),(XT(F7000510
I1),I#1,3) F7000520
750 FORMAT(IH 10X,A6,3H (I3,IH,I5,4H) 2F8.2,3X,3F8.3,1IX,3F8.4) F7000530
751 FORMAT(IH110X,I2A6) F7000540
752 FORMAT(IH110X,I8HSYMBOL ATOM CODE7X,16HPLOTTER X,Y(IN.) 3X,2IHCAF7000550
IRTESIAN X,Y,Z (IN.)15X,20HCRYSTAL SYSTEM X,Y,Z/IH 19X,45H(DIRECTIOF7000560
2N COSINES(I,J),I#1,3),RMSD(J)),J#1,3I2X,42HFOR PRINCIPAL AXES BASEF7000570
3D CN WORKING SYSTEM/IH ) F7000580
754 IF(EDGE-BRDR=.75)755,760,760 F7000590
755 NG#10 F7000600
756 CALL ERPNT(TI,730)
GO TO 1105 F7000610
760 IF(CHSYM)775,775,765 F7000620
C ***** PLOT CHEMICAL SYMBOLS *****
765 T4#1.
IF(VIEW)767,767,766 F7000640
766 T4#VIEW/(VIEW-X(3)) F7000650
767 T3#CHSYM*T4 F7000660
T4#DISP*T4*.5 F7000670
V1(1)#X(1)+DH*SYMB(1,1)+DV*SYMB(1,2) F7000680
V1(2)#X(2)+DH*SYMB(2,1)+DV*SYMB(2,2) F7000690
V1(3)#X(3) F7000700
CALL PLTXY(V1,V3) F7000710
IF(EDGE-CHSYM)775,768,768 F7000720
768 V2(3)#0.
DO 770 I#1,3,2 F7000730
V2(1)#V3(1)+FLOATF(I-2)*T4 F7000740
DO 770 J#1,3,2 F7000750
V2(2)#V3(2)+FLOATF(J-2)*T4 F7000760
CALL SIMBOL(V2(1),V2(2),T3,CHEM(K),THETA,6) F7000770
IF(T4)775,775,770 F7000780
770 CONTINUE F7000790
775 IF(NPLANE)1105,1105,780 F7000800
C ***** ELLIPSOID PRINC VECTORS TOWARD VIEWER *****
780 CALL PAXES(TI,2) F7000810
IF(NG)758,783,758 F7000820
783 CALL DIFV(EYE,XT,VIEWV) F7000830
CALL UNIT(VIEWV,VIEWV,-1) F7000840
CALL VM(VIEWV,AA,V2) F7000850
DO 795 I#1,3 F7000860
IF(VV(V2,PAT(I,I)))785,795,795 F7000870
785 DO 790 J#1,3 F7000880
PAC(J,I)#-PAC(J,I) F7000890
790 PAT(J,I)#-PAT(J,I) F7000900
795 CCNTINUE F7000910
DO 800 J#1,3 F7000920
PAC(J,4)#PAC(J,1) F7000930
800 PAC(J,5)#PAC(J,2) F7000940
IF(NJ2-I0)802,803,803 F7000950
801 FORMAT(IH 13X,3(3X,3F8.4,F8.5)/IH ) F7000960
802 WRITE OUTPUT TAPE NOUT,801,((PAC(J,K),J#1,3),RMS(K)),K#1,3) F7000970
C ***** V4 # VECTOR NORMAL TO POLAR PLANE *****
803 CALL VM(VIEWV,AAWRK,V6) F7000980
CALL UNIT(V6,V6,1) F7000990
CALL MV(Q,V6,V4) F7001000
CALL UNIT(V4,V4,1) F7001010
F7001020
F7001030
F7001040
F7001050
F7001060

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C **** SET PLOTTING RESOLUTION FOR ELLIPSOID **** F7001070
T3#RMS(3)*SCL F7001080
NRESOL#1 F7001090
NBIS#5 F7001100
DO 805 J#1,3 F7001110
IF(T3-RES(J))804,810,810 F7001120
804 NBIS#NBIS-1 F7001130
805 NRESOL#NRESOL*2 F7001140
810 NRESI#NRESOL+1 F7001150
C **** LOOP THROUGH PRINC AND POLAR PLANES **** F7001160
DO 1100 I#NFIRST,NPLANE F7001170
I10#XMODF(I1+2,3)+I F7001180
III#XMODF(I1,3)+I F7001190
II2#XMODF(I1+1,3)+I F7001200
C **** GENERATE CONJUGATE DIAMETERS **** F7001210
IF(.99938-ABSF(VV(V4,PAC(I,I12)))1820,820,830 F7001220
820 T1#RMS(I1)*SCL F7001230
T2#RMS(I11)*SCL F7001240
DO 825 J#1,3 F7001250
DA(J,1)#PAC(J,I10)*T1 F7001260
825 DA(J,2)#PAC(J,I11)*T2 F7001270
GO TO 850 F7001280
830 CALL NORM(PAC(I,I10),PAC(I,I11),VI,1) F7001290
CALL NORM(VI,V4,V2,1) F7001300
CALL UNIT(V2,V2,1) F7001310
CALL MV(Q,V2,V3) F7001320
IF(I1-4)835,840,840 F7001330
835 CALL NORM(V3,VI,V5,1) F7001340
GO TO 843 F7001350
840 CALL NORM(V3,V4,V5,1) F7001360
843 CALL UNIT(V5,V5,1) F7001370
T1#SCL/SQRTF(VMV(V2,Q,V2)) F7001380
T2#SCL/SQRTF(VMV(V5,Q,V5)) F7001390
DO 845 J#1,3 F7001400
DA(J,1)#V2(J)*T1 F7001410
845 DA(J,2)#V5(J)*T2 F7001420
C **** GENERATE ELLIPSE **** F7001430
850 CALL RADIAL(NBIS) F7001440
IF(I1-4)900,855,855 F7001450
C **** PLOT BOUNDARY ELLIPSE **** F7001460
855 CALL PRCJ(D,DP,X,X0,VIEW,1,129,NRESOL) F7001470
CALL DRAW(DP,0.,0.,3) F7001480
DO 860 J#NRES1,129,NRESOL F7001490
860 CALL DRAW(DP(1,J),0.,0.,2) F7001500
IF(DISP)1100,1100,865 F7001510
C **** BOUNDARY ANNULUS AS A LINEAR FUNCTION OF HEIGHT **** F7001520
865 CALL DIFV(XT,ORGN,VI) F7001530
T5#VV(VI,AAREV(I,3))*SCAL1 F7001540
NCYCLE#.5+(AIN(8)+T5*AIN(9))/DISP F7001550
IF(NCYCLE)1100,1100,870 F7001560
870 T3#(2.*DISP)/(T1+T2) F7001570
C **** INCREASE ANNULAR THICKNESS **** F7001580
DO 875 I#1,NCYCLE F7001590
T4#T3*FLOATF(I) F7001600
DO 875 J#1,129,NRESOL F7001610
875 CALL DRAW(DP(1,J),D(1,J)*T4,D(2,J)*T4,2) F7001620
GO TO 1100 F7001630
900 CALL PRCJ(D,DP,X,X0,VIEW,1,65,NRESOL) F7001640
C **** PLOT HALF AN ELLIPSE **** F7001650
CALL DRAW(DP,0.,0.,3) F7001660
DO 905 J#NRES1,65,NRESOL F7001670
905 CALL DRAW(DP(1,J),0.,0.,2) F7001680
IF(DISP)930,930,910 F7001690
C **** ACCENTUATE FRCNT HALF **** F7001700
910 DO 925 I#1,3,2 F7001710
T2#FLOATF(I-2)*DISP F7001720
DO 915 J#1,65,NRESOL F7001730
K#66-J F7001740
915 CALL DRAW(DP(1,K),DISP,T2,2) F7001750
DO 925 K#1,65,NRESOL F7001760

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925 CALL DRAW(DP(1,K),-DISP,-T2,2) F7001770
930 IF(NSOLID)940,967,935 F7001780
935 L#NDOT F7001790
  IF(NDOT-NRESOL)938,945,940 F7001800
938 CALL RADIAL(NSOLID-1) F7001810
  GO TO 945 F7001820
940 L#NRESOL F7001830
945 CALL PRCJ(D11,651,DP(1,651),X,X0,VIEW,1,65,L) F7001840
  IF(NSOLID)960,967,950 F7001850
C  ***** DOTTED LINE ON REVERSE SIDE *****
950 DO 958 J#65,129,NDOT F7001860
  CALL DRAW(DP(1,J),DISP,DISP,3) F7001870
  DO 955 I#1,3,2 F7001880
    T1#FLOATF(I-2)*DISP F7001890
  DO 955 K#1,3,2 F7001900
    T2#FLOATF(K-2)*DISP F7001910
  CALL DRAW(DP(1,J),T1,T2,2) F7001920
  IF(DISP)958,958,955 F7001930
955 CCNTINUE F7001940
958 CCNTINUE F7001950
  GO TO 967 F7001960
C  ***** SINGLE LINE ON REVERSE SIDE *****
960 DO 965 J#65,129,NRESOL F7001970
965 CALL DRAW(DP(1,J),0.,0.,2) F7001980
C  ***** DETAIL INTERIOR FEATURES *****
967 T2#NDASH#2 F7002000
  DO 975 J#1,3 F7002010
    T1#PAC(J,I10)*RMS(I10)*SCL F7002020
    DA(J,1)#T1 F7002030
    DA(J,2)#PAC(J,I11)*RMS(I11)*SCL F7002040
    DA(J,3)#D. F7002050
    IF(NDASH)975,975,970 F7002060
970 V1(J)#-T1 F7002070
  V2(J)#T1/T2 F7002080
975 CCNTINUE F7002090
  IF(NDASH)987,987,980 F7002100
C  ***** DASHED LINE FOR REVERSE AXIS *****
980 DO 985 J#1,NDASH F7002110
  DO 985 K#1,2 F7002120
  L#4-K F7002130
  CALL PRCJ(V1,DP,X,X0,VIEW,1,1,1) F7002140
  CALL DRAW(DP,0.,0.,L) F7002150
  DO 985 I#1,3 F7002160
  V1(I)#V1(I)+V2(I) F7002170
C  ***** SOLID LINE FOR FORWARD AXIS *****
987 IF(LINES)1100,1100,988 F7002180
988 CALL PRCJ(DA,DP,X,X0,VIEW,1,3,1) F7002190
  TI#DISP*.5 F7002200
  DO 990 I#1,3,2 F7002210
  T2#FLOATF(2-I)*T1 F7002220
  CALL DRAW(DP,T1,T2,3) F7002230
  CALL DRAW(DP(1,3),T1,T2,2) F7002240
  IF(DISP)1000,1000,989 F7002250
989 CALL DRAW(DP(1,3),-T1,T2,2) F7002260
990 CALL DRAW(DP,-T1,T2,2) F7002270
C  ***** SHADE QUADRANT BETWEEN TWO PRINCIPAL AXES *****
1000 L#LINES-1 F7002280
  IF(L)1100,1100,1005 F7002290
1005 T2#LINES F7002300
  DO 1025 I#1,L F7002310
    TI#FLOATF(I)/T2 F7002320
    T3#SQRTF(1.-T1*T1) F7002330
    IF(XMODF(I,2))1010,1015,1010 F7002340
1010 M#I*2 F7002350
  N#M-1 F7002360
  GO TO 1020 F7002370
1015 N#I*2 F7002380
  M#N-1 F7002390
1020 DO 1025 J#1,3 F7002400
  T4#DA(J,1)*T1 F7002410

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D(J,M)#T4 F7002470
1025 D(J,N)#DA(J,2)*T3+T4 F7002480
L#L*2 F7002490
CALL PROJ(D,DP,X,X0,VIEW,I,L,1) F7002500
DO 1030 I#2,L,2 F7002510
CALL DRAW(DP(I,I-1),0.,0.,3) F7002520
1030 CALL DRAW(DP(I,I),0.,0.,2) F7002530
1100 CCNTINUE F7002540
1105 CONTINUE F7002550
RETURN F7002560
END F7002570

*LIST8
*LABEL
      SUBROUTINE F800
C      **** SUBROUTINE FINDS ATOM PAIRS FOR BONDS **** F8000010
DIMENSION IA(3),WI(3) F8000020
DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F8000040
DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) F8000050
DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F8000060
DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F8000070
DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) F8000080
DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F8000090
DIMENSION XLNG(3),XO(3),XT(3) F8000100
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D F8000110
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F8000120
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI F8000130
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2 F8000140
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT F8000150
LNS#-4 F8000160
IF(XMODF(NJ2,10)-2)805,840,840 F8000170
C      **** EXPLICIT DESCRIPTION **** F8000180
 805 II#0 F8000190
  IF(NCD)845,845,815 F8000200
 815 II#II+1 F8000210
  IF(I40-II)899,899,820 F8000220
 820 TI#AIN(II) F8000230
  IF(TI)815,815,825 F8000240
 825 II#II+1 F8000250
  T2#AIN(II) F8000260
  IF(T2)815,815,830 F8000270
 830 IF(NJ2-10)832,838,838 F8000280
 832 LNS#XMODF(LNS+4,56) F8000290
  IF(LNS)838,834,838 F8000300
 834 WRITE OUTPUT TAPE NOUT,835,(TITLE(I),I#1,12) F8000310
 835 FORMAT(IH11OX,12A6) F8000320
  WRITE OUTPUT TAPE NOUT,837 F8000330
 837 FORMAT(IHDI0X,1BHSYMBOL ATOM CODE6X,16HPLOTTERR X,Y(IN.) 6X,2IHCAF8000340
  IRTESIAN X,Y,Z (IN.)17X,20HCRYSTAL SYSTEM X,Y,Z/IH ) F8000350
 838 CALL BOND(TI,T2,I) F8000360
  GO TO 815 F8000370
C      **** IMPLICIT DESCRIPTION **** F8000380
 840 IF(LATM-2)845,850,850 F8000390
 845 NG#I F8000400
  CALL ERPNT(0.,NJ*100+NJ2) F8000410
  GO TO 899 F8000420
 850 SCAL3#SCALI F8000430
  SCALI#1. F8000440
  DO 855 I#I,LATM F8000450
 855 CALL XYZ(ATOMS(I,I),ATOMS(2,I),2) F8000460
  SCALI#SCAL3 F8000470
  IF(NCD)845,845,860 F8000480
 860 WRITE OUTPUT TAPE NOUT,861 F8000490
 861 FORMAT(IHDI0X,20HBOND SELECTION CODES//IIX,94H(SEQUENCE(A))(SEQUENF8000500
  ICE(B)) (BCND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(F8000510
  2DIGITS) /IIX,93H( MIN MAX )( MIN MAX )( TYPE )( MIN MAX )(RADIF8000520
  3US)(HEIGHT OFFSET)(HEIGHT OFFSET)(NUMBER)) F8000530
  DMAX#0. F8000540
  DO 870 I#I,NCD F8000550
  IF(DMAX-CD(2,I))865,870,870 F8000560
 865 DMAX#CD(2,I) F8000570

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870 WRITE OUTPUT TAPE NOUT,871,(KD(J,I),J#1,5),(CD(J,I),J#1,8) F8000580
871 FORMAT(IH 10XI6,I5,I8,I5,I8,2F6.2,5F8.3,F7.0) F8000590
     DMAX#DMAX#DMAX F8000600
C      **** LCOP THROUGH ATOMS ARRAY **** F8000610
     DO 895 M#1,LATM F8000620
     TI#ATOMS(1,M) F8000630
     IA(1)#TI/100000. F8000640
     IA(3)#IA(1) F8000650
     WI(1)#ATOMS(2,M) F8000660
     WI(2)#ATOMS(3,M) F8000670
     WI(3)#ATOMS(4,M) F8000680
     L#M+1 F8000690
     DO 895 N#L,LATM F8000700
     DIST#(ATOMS(2,N)-WI(1))**2 F8000710
     IF(DMAX-DIST)895,873,873 F8000720
873 DIST#DIST+(ATOMS(3,N)-WI(2))**2 F8000730
     IF(DMAX-DIST)895,874,874 F8000740
874 DIST#DIST+(ATOMS(4,N)-WI(3))**2 F8000750
     IF(DMAX-DIST)895,875,875 F8000760
875 DIST#SQRTF(DIST) F8000770
     T2#ATOMS(1,N) F8000780
     IA(2)#T2/100000. F8000790
C      **** SELECT BONDS ACCORDING TO CODES **** F8000800
     DO 890 J#1,NCD F8000810
     JB#J F8000820
     IF(DIST-CD(I,J)) 890,880,880 F8000830
880 IF(CD(2,J)-DIST) 890,881,881 F8000840
881 DO 885 K#1,2 F8000850
     IF(IA(K)-KD(I,J)) 885,882,882 F8000860
882 IF(KD(2,J)-IA(K)) 885,883,883 F8000870
883 IF(IA(K+1)-KD(3,J))885,884,884 F8000880
884 IF(KD(4,J)-IA(K+1))885,891,891 F8000890
885 CONTINUE F8000900
890 CONTINUE F8000910
     GO TO 895 F8000920
891 IF(NJ2-I0)892,894,894 F8000930
892 LNS#XMODF(LNS+4,56) F8000940
     IF(LNS)893,893,894 F8000950
893 WRITE OUTPUT TAPE NOUT,835,(TITLE(I),I#1,12) F8000960
     WRITE OUTPUT TAPE NOUT,837 F8000970
894 CALL BOND(T1,T2,JB) F8000980
895 CCNTINUE F8000990
899 RETURN F8001000
     END F8001010

*LIST8
*LABEL
      SUBROUTINE F900 F9000010
      DIMENSION X(3),XW(3,5),Y(3),Z(3) F9000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) F9000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F9000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F9000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F9000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) F9000070
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) F9000080
      DIMENSION XLNG(3),XO(3),XT(3) F9000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,RR,BRDR,CD,CHEM,CONT,D F9000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F9000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI F9000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 F9000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT F9000140
      **** LABELING FUNCTION SUBROUTINE **** F9000150
     ITILT#0 F9000160
     NJ3#XMODF(NJ2,I0) F9000170
     TH#THETA F9000180
     SINTH#SYMB(2,1) F9000190
     COSTH#SYMB(1,1) F9000200
     ILAST#1 F9000210
     IF(AIN(2)-11100.)910,910,905 F9000220
905 ILAST#2 F9000230
910 DO 925 II#1,ILAST F9000240

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C ***** OBTAIN WORKING CARTESIAN COORDINATES *****
CALL XYZ(AIN(II),XW(I,II),2) F9000250
IF(NG)915,925,915 F9000260
912 NG#15 F9000270
915 CALL ERPNT(AIN(II),NJ*100+NJ2) F9000280
GO TO 1199 F9000290
925 CALL XYZ(AIN(II),XW(I,II+3),3) F9000300
II#1 F9000310
C ***** FIND MEAN REFERENCE POINT *****
DO 930 J#1,3 F9000320
T2#XW(J,ILAST) F9000330
TI#XW(J,1) F9000340
XW(J,3)#T2-TI F9000350
930 X(J)#{T2+TI}*5 F9000360
F9000370
C ***** PERSPECTIVE SCALING FACTOR *****
SCAL#1. F9000380
IF(VIEW)940,940,935 F9000390
935 SCAL#VIEW/(VIEW-X(3)) F9000400
940 HGT#SCAL*AIN(5) F9000410
IF(NJ2-3)960,950,945 F9000420
945 IF(NJ2-6)950,950,960 F9000430
F9000440
C ***** PROJECTED VECTOR BASELINE *****
950 CALL PLTXY(XW(I,4),V1) F9000450
CALL PLTXY(XW(I,5),V2) F9000460
T1#V2(1)-V1(1) F9000470
T2#V2(2)-V1(2) F9000480
T3#SQRTF(T1*T1+T2*T2) F9000490
IF(T3)912,912,955 F9000500
955 COSTH#T1/T3 F9000510
SINTH#T2/T3 F9000520
TH#ARCCOS(COSTH) F9000530
IF(SINTH)958,960,960 F9000540
958 TH#-TH F9000550
F9000560
960 IF(NJ2-13)965,985,985 F9000570
C ***** FIND CENTER OF PROJECTED LABEL *****
965 Y(1)#SCAL*(X(1)+AIN(6)*COSTH-AIN(7)*SINTH)+XO(1) F9000580
Y(2)#SCAL*(X(2)+AIN(6)*SINTH+AIN(7)*COSTH)+XO(2) F9000590
Y(3)#0. F9000600
970 TH#-TH F9000610
F9000620
C ***** CHECK FOR LEGEND RESET *****
DO 980 J#1,2 F9000630
T1#AIN(J+2) F9000640
IF(T1)975,980,970 F9000650
970 Y(J)#T1 F9000660
GO TO 980 F9000670
975 Y(J)#XLNG(J)+T1 F9000680
980 CONTINUE F9000690
F9000700
C ***** SET PARAMETERS FOR INDIVIDUAL FUNCTIONS *****
985 GO TO(990,995,995,1000,1000,1000,915,1105,1105,915,915,915,1005,10F9000720
105,1005,1005,915),NJ2 F9000730
990 T6#17. F9000740
L#AIN(1)/100000. F9000750
ILAST#1 F9000760
DXW#0. F9000770
DYW#0. F9000780
GO TO 1030 F9000790
995 T6#215. F9000800
ILAST#12 F9000810
T1#HGT*36./7. F9000820
DXW#COSTH*T1 F9000830
DYW#SINTH*T1 F9000840
GO TO 1030 F9000850
1000 T6#22+3*(6-NJ3) F9000860
DIST#SQRTF(VV(XW(I,3),XW(I,3)))/SCAL I F9000870
GO TO 1030 F9000880
C ***** TRUE PERSPECTIVE LABELS *****
1005 CALL UNIT(XW(I,3),VT(I,1),1) F9000890
IF(ABSF(VT(3,1))-9994)1010,912,912 F9000900
C ***** FORM PERSPECTIVE ROTATION MATRIX *****
1010 CALL NORM(AID(I,3),VT(1,1),VT(1,2),1) F9000910
CALL UNIT(VT(1,2),VT(1,2),1) F9000920
F9000930
F9000940

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      CALL NORM(VT(1,1),VT(1,2),VT(1,3),1)          F9000950
      DO 1015 J#1,3                                F9000960
1015 VT(J,4)#X(J)                                F9000970
      ITILT#1                                     F9000980
      HGT#AIN(5)                                  F9000990
      TH#0.                                      F9001000
      Y(3)#X(3)                                  F9001010
      Y(2)#X(2)+AIN(7)-HGT*.5                  F9001020
      IF(NJ2-13)1030,1025,1020                  F9001030
C      ***** PERSPECTIVE BCND LABELS *****       F9001040
1020 Y(1)#X(1)+AIN(6)-HGT*FLOATF(22+3*(6-NJ3))/7. F9001050
      DIST#SQRTF(VV(XW(1,3),XW(1,3)))/SCAL1      F9001060
      GO TO 1050                                  F9001070
C      ***** PERSPECTIVE TITLES *****            F9001080
1025 Y(1)#X(1)+AIN(6)-HGT*215./7.             F9001090
      ILAST#12                                 F9001100
      DXW#HGT*36./7.                           F9001110
      DYW#0.                                    F9001120
      GO TO 1050                                 F9001130
1030 DH#HGT*T6/7.                            F9001140
      DV#HGT*.5                               F9001150
      Y(1)#Y(1)-DH*COSTH+DV*SINTH            F9001160
      Y(2)#Y(2)-DH*SINTH-DV*COSTH           F9001170
      Y(3)#0.                                    F9001180
C      ***** PLOT VARIOUS LABELS *****          F9001190
1050 GO TO(1060,1060,1060,1090,1095,1100,915,1105,1105),NJ3 F9001200
1060 DO 1085 I#1,ILAST                      F9001210
      DO 1075 J#1,3,2                          F9001220
      Z(1)#Y(1)+FLOATF(J-2)*DISP*.5        F9001230
      DO 1075 K#1,3,2                          F9001240
      Z(2)#Y(2)+FLOATF(K-2)*DISP*.5        F9001250
      IF(NJ3-2)1065,1068,1068                  F9001260
C      ***** PLOT CHEMICAL SYMBOL *****        F9001270
1065 CALL SIMBOL(Z(1),Z(2),HGT,CHEM(L),TH,6) F9001280
      GO TO 1070                                F9001290
C      ***** PLOT TITLES *****                 F9001300
1068 CALL SIMBOL(Z(1),Z(2),HGT,TITLE2(I),TH,6) F9001310
1070 IF(DISP)1080,1080,1075                  F9001320
1075 CONTINUE                                F9001330
1080 Y(1)#Y(1)+DXW                         F9001340
1085 Y(2)#Y(2)+DYW                         F9001350
      GO TO 1199                                F9001360
C      ***** PLOT BCND DISTANCE LABELS *****   F9001370
1090 CALL NUMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.1) F9001380
      GO TO 1199                                F9001390
1095 CALL NUMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.2) F9001400
      GO TO 1199                                F9001410
1100 CALL NUMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.3) F9001420
      GO TO 1199                                F9001430
C      ***** PLOT CENTERED SYMBOLS *****        F9001440
1105 CALL SIMBOL(Y(1),Y(2),HGT,XFIXF(AIN(8)),TH,7-NJ3) F9001450
1199 ITILT#0
      RETURN
      END

*LIST8
*LABEL
      SUBROUTINE F1000                         F10C0010
      RETURN
      END
*LIST8
*LABEL
      SUBROUTINE MM(X,Y,Z)                      MM  0010
C      MULTIPLY TWO MATRICES                  MM  0020
C      Z(3,3)#X(3,3)*Y(3,3)                  MM  0030
      DIMENSIONX(3,3),Y(3,3),Z(3,3)          MM  0040
      DO117I#1,3                                MM  0050
      DO117K#1,3                                MM  0060
      Z(I,K)#0.0                                MM  0070
      DO117J#1,3                                MM  0080
117 Z(I,K)#Z(I,K)+X(I,J)*Y(J,K)          MM  0090

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      RETURN                               MM 0100
      END                                 MM 0110
*LIST8
*LABEL
      SUBROUTINE MV(X,Y,Z)                MV 0010
C      MATRIX * VECTOR                  MV 0020
C      Z(3)*X(3,3)*Y(3)                 MV 0030
      DIMENSION X(3,3),Y(3),Z(3)          MV 0040
      DO113I#1,3                         MV 0050
      Z(I)#0.0                           MV 0060
      DO113J#1,3                         MV 0070
113 Z(I)*Z(J)+X(I,J)*Y(J)           MV 0080
      RETURN                               MV 0090
      END                                 MV 0100
*LIST8
*LABEL
      SUBROUTINE NORM(X,Y,Z,ITYPE)        NORM0010
C      ***** VECTOR PRODUCT Z*X*Y *****   NORM0020
C      ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****
      DIMENSION X(3),Y(3),Z(3,3),Z1(3,3)  NORM0040
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) NORM0050
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) NORM0060
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) NORM0070
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) NORM0080
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  NORM0090
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) NORM0100
      DIMENSION XLNG(3),XO(3),XT(3)       NORM0110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D NORM0120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD NORM0130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI NORM0140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 NORM0150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT NORM0160
      DO I25 I#1,3                      NORM0170
      I1#XMODF(I+3,3)+1                 NORM0180
      I2#XMODF(I+1,3)+1                 NORM0190
      T1#X(I)*Y(I2)-X(I2)*Y(I1)       NORM0200
      IF(ITYPE)115,115,105             NORM0210
105 Z(I)#T1                          NORM0220
      GO TO I25                         NORM0230
115 Z1(I)#T1                         NORM0240
125 CCNTINUE                         NORM0250
      IF(ITYPE)135,135,300              NORM0260
135 CALL MV(BB,Z1,Z)                 NORM0270
300 RETURN                            NORM0280
      END                                NORM0290
*LIST8
*LABEL
      SUBROUTINE PAXES(ACODE,ITYPE)       PAXE0010
C      ***** ITYPE .LT.0 FOR COVARIANCE MATRIX IN Q *****
C      ***** ITYPE .GT.0 FOR ELLIPSOID QUADRATIC FORM IN Q *****
C      ***** XABSF(ITYPE)#1 BASED ON TRICLINIC COORDINATE SYSTEM *****
C      ***** #2 OR 3 FOR WORKING OR REFERENCE CARTESIAN SYSTEMS *****
C      ***** CHECK ATOM CODE *****
      DIMENSION W(3,3),X(3)              PAXE0070
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) PAXE0080
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) PAXE0090
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PAXE0100
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PAXE0110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  PAXE0120
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) PAXE0130
      DIMENSION XLNG(3),XO(3),XT(3)       PAXE0140
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D PAXE0150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PAXE0160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI PAXE0170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 PAXE0180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT PAXE0190
      IT#XABSF(ACODE)-1                 PAXE0200
      KS#MODF(ACODE,100.)               PAXE0210
      IF(NSYM-KS)105,115,115            PAXE0220
105 NG#4                                PAXE0230

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      GO TO 300
115 I#ACODE/100000.
      IF(NATOM-II)125,130,130
125 NG#5
      GO TO 300
130 IF(II)125,125,135
C      ***** CRYSTALLOGRAPHIC SYMMETRY ROTATION *****
135 CALL TMM(PA(I,I,II),FS(I,I,KS),PAT)
      IF(IT-I)165,145,155
C      ***** TRANSFORM TO CARTESIAN SYSTEMS *****
145 CALL TMM(PAT,AAWRK,PAC)
      GO TO 175
155 CALL TMM(PAT,AAREV,PAC)
      GO TO 175
165 IF(IITYPE)170,175,170
C      ***** (PAT)**(-1) * (AA)**(-1) *****
170 CALL AXEQB(PAT,W,BB,3)
C      ***** FORM DIAGONAL MATRIX OR ITS INVERSE *****
175 DO 205 J#I,3
      TI#EV(J,II)
      IF(IITYPE)195,205,185
185 X(J)#1./(TI*T)
      GO TO 205
195 X(J)#TI*T
205 RMS(J)#TI
C      ***** FORM QUADRATIC FORM *****
      DO 245 I#I,3
      DO 245 J#I,3
      TI#0.0
      IF(IT)300,210,220
210 DO 215 K#I,3
C      ***** BASED ON TRICLINIC SYSTEM *****
215 TI#TI+PAT(I,K)*W(K,J)*X(K)
      GO TO 235
C      ***** BASED ON CARTESIAN SYSTEM *****
220 DO 225 K#I,3
225 TI#TI+PAC(I,K)*PAC(J,K)*X(K)
235 Q(J,I)#TI
245 Q(I,J)#TI
300 RETURN
      END
*LIST8
*LABEL
      SUBROUTINE PLTXY(X,Y)
C      ***** PLOT COORD. AND CLOSEST EDGE AFTER PROJECTION *****
      DIMENSION X(3),Y(2)
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) PLTX0010
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) PLTX0020
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(31) PLTX0030
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PLTX0040
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) PLTX0050
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) PLTX0060
      DIMENSION XLNG(3),XO(3),XT(3) PLTX0070
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D PLTX0080
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PLTX0090
      COMMON NJ,NJ2,NOUT,NSR,NSYM,CRGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI PLTX0100
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 PLTX0110
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      T4#1.
      T1#1.
      IF(VIEW)125,125,110
110 T4#VIEW-X(3)
      IF(T4)115,115,120
115 Y(1)#-99.
      Y(2)#-99.
      GO TO 130
120 T1#VIEW/T4
125 Y(1)#X(1)*T1+X0(1)
      Y(2)#X(2)*T1+X0(2)
      T1#XLNG(1)-ABSF(Y(1)*2.-XLNG(1)) PLTX0120
PLTX0130
PLTX0140
PLTX0150
PLTX0160
PLTX0170
PLTX0180
PLTX0190
PLTX0200
PLTX0210
PLTX0220
PLTX0230
PLTX0240
PLTX0250
PLTX0260
PLTX0270
PLTX0280
PLTX0290
PLTX0300
PLTX0310
PLTX0320
PLTX0330
PLTX0340
PLTX0350
PLTX0360
PLTX0370
PLTX0380
PLTX0390
PLTX0400
PLTX0410
PLTX0420
PLTX0430
PLTX0440
PLTX0450
PLTX0460
PLTX0470
PLTX0480
PLTX0490
PLTX0500
PLTX0510
PLTX0520
PLTX0530
PLTX0540
PLTX0550
PLTX0560
PLTX0570
PLTX0580
PLTX0590
PLTX0600
PLTX0610
PLTX0620
PLTX0630
PLTX0640
PLTX0010
PLTX0020
PLTX0030
PLTX0040
PLTX0050
PLTX0060
PLTX0070
PLTX0080
PLTX0090
PLTX0100
PLTX0110
PLTX0120
PLTX0130
PLTX0140
PLTX0150
PLTX0160
PLTX0170
PLTX0180
PLTX0190
PLTX0200
PLTX0210
PLTX0220
PLTX0230
PLTX0240
PLTX0250
PLTX0260
PLTX0270

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T2#XLNG(2)-ABSF(Y(2)*2.-XLNG(2))          PLTX0280
EDGE#MINIF(T1,T2)*.5                         PLTX0290
IF(T4-VIEW*.5)I30,300,300                     PLTX0300
130 EDGE#-99.                                 PLTX0310
301 RETURN.                                  PLTX0320
END                                         PLTX0330

*LIST8
*LABEL
      SUBROUTINE PRELIM                      PREL0010
C      ***** DATA INPUT ROUTINE *****        PREL0020
DIMENSION B(9)                                PREL0030
DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) PREL0040
DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PREL0050
DIMENSION DA(3,31),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PREL0060
DIMENSION P(3,200),PA(3,3,20C),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PREL0070
DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  PREL0080
DIMENSION VT(3,41),V1(4),V2(3),V3(3),V4(31),V5(3),V6(3),WRKV(3,3) PREL0090
DIMENSION XLNG(31),XO(31),XT(3)                PREL0100
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  PREL0110
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PREL0120
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI PREL0130
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2  PREL0140
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT            PREL0150
C      ***** CELL DIMENSIONS *****           PREL0160
106 FORMAT(6F9.6)                            PREL0170
READ INPUT TAPE IN,106,(A(I),I#1,6)
T1#ABSF(A(4))-1.                           PREL0180
DO 125 J#1,3                               PREL0190
IF(T1)I15,I10,I10                         PREL0200
C      ***** CELL ANGLES IN DEGREES *****    PREL0210
110 A(J+6)#A(J+3)                          PREL0220
A(J+3)#COSF(A(J+6)*.01745329252)        PREL0230
GO TO 120                                  PREL0240
C      ***** COSINES OF CELL ANGLES *****   PREL0250
115 A(J+6)#ARCCOS(A(J+3))                 PREL0260
C      ***** STORE IDEMFACTOR MATRIX *****   PREL0270
120 AID(J,J)#1.                           PREL0280
AID(J+1,1)#0.                           PREL0290
AID(J+5,1)#0.                           PREL0300
C      ***** STORE METRIC TENSOR *****       PREL0310
125 AA(J,J)#A(J)**2                      PREL0320
AA(1,2)#A(1)*A(2)*A(6)                  PREL0330
AA(1,3)#A(1)*A(3)*A(5)                  PREL0340
AA(2,3)#A(2)*A(3)*A(4)                  PREL0350
AA(2,1)#AA(1,2)                         PREL0360
AA(3,1)#AA(1,3)                         PREL0370
AA(3,2)#AA(2,3)                         PREL0380
C      ***** INVERT METRIC TENSOR *****     PREL0390
CALL AXEQB(AA,BB,AID,3)                  PREL0400
C      ***** CALCULATE RECIPROCAL CELL PARAMETERS *****  PREL0410
C      ***** DO 128 J#1,3                   PREL0420
DO 128 B(J)#SQRTF(BB(J,J))
B(6)#BB(1,2)/(B(1)*B(2))                PREL0430
B(5)#BB(1,3)/(B(1)*B(3))                PREL0440
B(4)#BB(2,3)/(B(2)*B(3))                PREL0450
DO 130 J#1,3
130 B(J+6)#ARCCOS(B(J+3))               PREL0460
C      ***** WAS INPUT FOR REAL OR RECIPROCAL CELL *****  PREL0470
IF(A(1)-1.)I35,150,150
135 DO 140 J#1,9
T1#AA(J,1)
AA(J,1)#BB(J,1)
BB(J,1)#T1
T1#A(J)
A(J)#B(J)
140 B(J)#T1
C      ***** WRITE OUT CELL PARAMETERS *****  PREL0480
143 FORMAT(IH010X,22HDIRECT CELL PARAMETERS/IH 15X,1HA14X,1HB14X,1HC14PREL0490
IX,5HALPHA10X,4HBETAIIX,5HGAMMA)        PREL0500
145 FORMAT(IH 10X,F9.6,2F15.6,3F15.3/IH 48X,6HCOSINEF 12.8,2F15.8)  PREL0510

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147 FORMAT(IH10X,26HRECIPROCAL CELL PARAMETERS/IH 15X,2HA*13X,2HB*13XPREL0630
1,2HC*13X,6HALPHA*9X,5HBETA*10X,6HGAMMA*) PREL0640
150 WRITE OUTPUT TAPE NOUT,143 PREL0650
    WRITE OUTPUT TAPE NOUT,145,(A(I),I#1,3),(A(I),I#7,9),(A(I),I#4,6) PREL0660
    WRITE OUTPUT TAPE NOUT,147 PREL0670
    WRITE OUTPUT TAPE NOUT,145,(B(I),I#1,3),(B(I),I#7,9),(B(I),I#4,6) PREL0680
C    **** STORE STANDARD VECTORS **** PREL0690
    CALL AXES(AID,AID(1,2),REFV,0) PREL0700
    CALL MM(AA,REFV,AAREV) PREL0710
    DO 160 I#1,3 PREL0720
    DO 160 J#1,3 PREL0730
    AAWRK(J,I)#AAREV(J,I) PREL0740
    Q(J,I)#REFV(I,J) PREL0750
160 WRKV(J,I)#REFV(J,I) PREL0760
C    **** READ AND WRITE SYMMETRY TRANSFORMATIONS **** PREL0770
171 FORMAT(IH10X,24HSYMMETRY TRANSFORMATIONS/IH 14X,3HNO.12X,13HTRANSPREL0780
1F1M0ED X18X,13HTRANSFORMED Y18X,13HTRANSFORMED Z) PREL0790
173 FORMAT(II,FI4.10,3F3.0,2(F15.10,3F3.0)) PREL0800
175 FORMAT(IH 13X,I2,3(F13.6,F4.0,2H XF4.0,2H YF4.0,2H Z)) PREL0810
177 FORMAT(IH110X,I2A6) PREL0820
    WRITE OUTPUT TAPE NOUT,171 PREL0830
    LINES#14 PREL0840
    DO 190 I#1,48 PREL0850
    LINES#XMODF(LINES+1,56) PREL0860
    READ INPUT TAPE IN,173,IS,(TS(J,I),(FS(K,J,I),K#1,3),J#1,3) PREL0870
    IF(LINES)185,180,185 PREL0880
180 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12) PREL0890
    WRITE OUTPUT TAPE NOUT,171 PREL0900
185 WRITE OUTPUT TAPE NOUT,175,I,(TS(J,I),(FS(K,J,I),K#1,3),J#1,3) PREL0910
C    **** NCN-CRYSTALLOGRAPHIC HELIX-SYMMETRY INPUT **** PREL0920
    IF(FS(3,3,I)-5.)188,186,186 PREL0930
186 T1#FS(1,3,I)/FS(3,3,I) PREL0940
    TS(3,I)#TS(3,I)+T1 PREL0950
    T1#MODF(T1*FS(2,3,I),1.)*6.28318531 PREL0960
    T2#COSF(T1) PREL0970
    T1#SINF(T1) PREL0980
    DO 187 J#1,9 PREL0990
187 VT(J,I)#AID(J,I) PRELI000
    VT(1,1)#T2 PRELI010
    VT(2,2)#T2 PRELI020
    VT(2,1)#-T1 PRELI030
    VT(1,2)#T1 PRELI040
    CALL MM(VT,Q,PAC) PRELI050
    CALL MM(AAREV,PAC,FS(1,1,I)) PRELI060
188 IF(IS)195,190,195 PRELI070
190 CONTINUE PRELI080
    NG#1 PRELI090
    CALL ERPNT(0.,0) PRELI100
    I#48 PRELI110
195 NSYM#1 PRELI120
C    **** POSITIONAL AND THERMAL PARAMETERS **** PRELI130
207 FORMAT(IH10 NO. ATOM 8X,1HX10X,1HY10X,1HZ13X,3HB118X,3HB228X,3HB33PREL1140
18X,3HB128X,3HB138X,10HB23 TYPE) PRELI1150
209 FORMAT(IH 13,1X,A6,3F11.6,5X,6F11.6,F5.0) PRELI1160
210 FORMAT(IH 13,1X,A6,3F11.6,5X,2F11.6,4F11.0,F5.0) PRELI1170
211 FORMAT(A6,3X,5F9.6,F9.0) PRELI1180
213 FORMAT(II,F8.6,5F9.6,F9.0) PRELI1190
    LINES#LINES+2 PRELI1200
    IF(LINES-56)220,215,215 PRELI1210
215 LINES#-1 PRELI1220
    GO TO 225 PRELI1230
220 WRITE OUTPUT TAPE NOUT,207 PRELI1240
225 DO 245 I#1,200 PRELI1250
    LINES#XMODF(LINES+1,56) PRELI1260
    READ INPUT TAPE IN,211,CHEM(I),VI(1),VI(2),(P(J,I),J#1,3),TI PRELI1270
    K#1.+TI PRELI1280
    READ INPUT TAPE IN,213,IS,(PA(J,I,I),J#1,7) PRELI1290
    IF(LINES)230,230,232 PRELI1300
230 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12) PRELI1310
    WRITE OUTPUT TAPE NOUT,207 PRELI1320

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232 IF(PA(3,I,I)-10000.1235,234,234 PREL1330
234 WRITE OUTPUT TAPE NOUT,210,I,CHEM(I),(P(J,I),J#1,3),(PA(J,I,I),J#I)PREL1340
1,7) PREL1350
GO TO 238 PREL1360
235 WRITE OUTPUT TAPE NOUT,209,I,CHEM(I),(P(J,I),J#1,3),(PA(J,I,I),J#I)PREL1370
1,7) PREL1380
238 GO TO (244,239,241,242,244),K PREL1390
C **** TYPE 1 POSITIONAL PARAMETERS (ANGSTROMS) **** PREL1400
239 DO 240 J#1,3 PREL1410
240 P(J,I)*P(J,I)/A(J) PREL1420
GO TO 244 PREL1430
C **** TYPE 2 POSITIONAL PARAMETERS, STANDARD CARTESIAN **** PREL1440
241 VI(1)*P(1,I) PREL1450
VI(2)*P(2,I) PREL1460
GO TO 243 PREL1470
C **** TYPE 3 POSITIONAL PARAMETERS **** PREL1480
C **** CYLINDRICAL COORDINATES REFERRED TO STANDARD CARTESIAN **** PREL1490
242 T2#P(2,I)*.01745329252 PREL1500
VI(1)*VI(1)+P(1,I)*COSF(T2) PREL1510
VI(2)*VI(2)+P(1,I)*SINF(T2) PREL1520
243 VI(3)*P(3,I) PREL1530
CALL VM(VI,Q,P(I,I)) PREL1540
244 IF(IS)246,245,246 PREL1550
245 CONTINUE PREL1560
NG#2 PREL1570
CALL ERPNT(0.,0) PREL1580
I#200 PREL1590
246 NATOM#I PREL1600
C **** CONVERT TEMP FACTOR COEF TO STANDARD TYPE ZERO **** PREL1610
NG1#0 PREL1620
DO 450 I#1,NATOM PREL1630
TI#PA(1,I,I) PREL1640
K#I.+PA(7,I,I) PREL1650
IF(TI)250,250,255 PREL1660
250 TI#.I PREL1670
GO TO 405 PREL1680
255 T6#.0506605918 PREL1690
GO TO(270,260,265,265,270,260,400,405,999),K PREL1700
C **** TYPE 1 **** PREL1710
260 DO 262 J#4,6 PREL1720
262 PA(J,I,I)*PA(J,I,I)*.5 PREL1730
GO TO 270 PREL1740
C **** TYPES 2 AND 3 (BASE 2 SYSTEMS) **** PREL1750
265 T6#.351152464 PREL1760
IF(K-4)270,260,270 PREL1770
C **** TYPES 0 THROUGH 5 **** PREL1780
270 IF(PA(2,I,I))400,400,272 PREL1790
272 DO 300 J#1,3 PREL1800
DO 300 L#J,3 PREL1810
T2#T6 PREL1820
IF(K-5)285,275,275 PREL1830
C **** TYPES 4 AND 5 **** PREL1840
275 T2#B(J)*B(L)*T2*.25 PREL1850
285 IF(J-L)290,282,290 PREL1860
282 VT(J,J)*T2*PA(J,I,I) PREL1870
GO TO 300 PREL1880
290 M#J+L+1 PREL1890
VT(J,L)*T2*PA(M,I,I) PREL1900
VT(L,J)*VT(J,L) PREL1910
300 CCNTINUE PREL1920
C **** FIND PRINCIPAL AXES **** PREL1930
CALL MM(VT,AA,DA) PREL1940
CALL EIGEN(DA,RMS,PAT) PREL1950
C **** ARE EIGENVALUES POSITIVE **** PREL1960
IF(RMS(I))325,325,320 PREL1970
320 IF(NG)350,360,330 PREL1980
325 NG#3 PREL1990
330 NG#I PREL2000
CALL ERPNT(FLOATF(I)*100000.+55501.,0) PREL2010
C **** 3 EQUAL EIGENVALUES, USE REFERENCE VECTORS **** PREL2020

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340 T3#SIGNF(SQRTF(ABSF(RMS(1)+RMS(2)+RMS(3))/3.),RMS(1)) PREL2030
    DO 345 J#1,3
    DO 342 K#1,3
342 PA(J,K,I)#REFV(J,K) PREL2040
345 EV(J,T)#T3 PREL2050
    GO TO 450 PREL2060
350 IF(NG+6)340,340,352 PREL2070
C     ***** TWO EQUAL EIGENVALUES *****
352 N#NG+5 PREL2080
    CALL UNIT(PAT(I,N),VI,-1)
    DO 354 K#1,3
        IF(ABSF(VMV(VI,AA,REFV(I,K)))-.58)356,354,354 PREL2090
354 CONTINUE PREL2100
356 CALL MM(AA,DA,VT) PREL2110
    CALL AXES(VI,REFV(I,K),DA,-1)
    DO 359 K#1,3
        L#XMODF(N#K-2,3)+I PREL2120
    DO 358 J#1,3
358 PA(J,L,I)#DA(J,K) PREL2130
359 EV(L,I)#SIGNF(SQRTF(ABSF(VMV(DA(I,K),VT,DA(I,K)))),RMS(L)) PREL2140
    GO TO 450 PREL2150
C     ***** MAKE EIGENVECTORS I ANGSTROM LONG *****
360 DO 365 J#1,3 PREL2160
365 CALL UNIT(PAT(I,J),PA(I,J,I),-1) PREL2170
370 NG#0 PREL2180
C     ***** SQRT EIGENVALUE # RMS DISPLACEMENT *****
    DO 375 J#1,3 PREL2190
        T2#RMS(J)
375 EV(J,I)#SIGNF(SQRTF(ABSF(T2)),T2) PREL2200
    GO TO 450 PREL2210
C     ***** TYPE 6 (ISOTROPIC TEMP FACTOR) *****
400 TI#SQRTF(TI*.D12665148) PREL2220
C     ***** TYPE 7 (DUMMY SPHERE) *****
405 DO 410 J#1,3 PREL2230
410 EV(J,I)#TI PREL2240
    IF(PA(3,I,I))430,430,415 PREL2250
C     ***** DEFINED VECTORS FOR SPHERE *****
415 DO 425 J#1,4 PREL2260
    T2#PA(J+2,I,I)
    CALL ATOM(T2,VT(I,J))
    IF(NG)420,425,420 PREL2270
420 CALL ERPNT(T2,0) PREL2280
    GO TO 430 PREL2290
425 CCNTINUE PREL2300
    CALL DIFV(VT(1,2),VT(1,1),VI)
    CALL DIFV(VT(1,4),VT(1,3),V2)
    CALL AXES(VI,V2,PA(I,I,I),-1)
    GO TO 450 PREL2310
C     ***** REFERENCE VECTORS FOR SPHERE *****
430 DO 435 J#1,9 PREL2320
435 PA(J,I,I)#REFV(J,I) PREL2330
450 NG#0 PREL2340
C     ***** WRITE OUT RMS VALUES *****
    LINES#LINES+2 PREL2350
    IF(LINES-56)458,458,455 PREL2360
455 LINES#-1 PREL2370
    GO TO 460 PREL2380
458 WRITE OUTPUT TAPE NOUT,461 PREL2390
460 DO 465 I#1,NATOM PREL2400
    LINES#XMODF(LINES+1,56)
    IF(LINES)465,462,465 PREL2410
461 FORMAT(I0H0NO. ATOM BX,1HX10X,1HY10X,1HZ13X,7HRMSD 1 4X,7HRMSD 2 4PREL2420
    IX,7HRMSD 3 ) PREL2430
462 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12) PREL2440
    WRITE OUTPUT TAPE NOUT,461 PREL2450
463 FORMAT(1H I3,IX,A6,3F11.6) PREL2460
465 WRITE OUTPUT TAPE NOUT,209,I,CHEM(I),(P(J,I),J#1,3),(EV(J,I),J#1,3PREL2470
    I)
    IF(NG)999,999,470 PREL2480
470 CALL EXIT PREL2490

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999 RETURN
END
*LIST8
*LABEL
      SUBROUTINE PRIME
C      ****GENERAL INITIALIZATION OF PRIME PARAMETERS****
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) PRIM0010
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) PRIM0020
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PRIM0030
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PRIM0040
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) PRIM0050
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) PRIM0060
      DIMENSION XLNG(3),XO(3),XT(3) PRIM0070
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D PRIM0080
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,LATM,LTNO,NATOM,NCD PRIM0090
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI PRIM0100
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 PRIM0110
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT PRIM0120
      BRDR#0.5 PRIM0130
C      ****CALCULATE CONSTANTS****
      DO 2999 I#1,5 PRIM0140
2999 CONT(I)#SQRTF(1./(2.*(.+COSF(3.141592654/2.*I)))) PRIM0150
      DISP#.005 PRIM0160
      FORE#.866 PRIM0170
      IN#10 PRIM0180
      ITILT#0 PRIM0190
      LATM#0 PRIM0200
      LTNO#23 PRIM0210
      NCD#0 PRIM0220
      NG#0 PRIM0230
      NOUT#9 PRIM0240
      NSR#11 PRIM0250
      RES(I)#1.25 PRIM0260
      RES(2)#.5 PRIM0270
      RES(3)#.2 PRIM0280
      SCAL1#1.0 PRIM0290
      SCAL2#1.54 PRIM0300
      SCL#1.54 PRIM0310
      DO 3000 I#1,3 PRIM0320
      SYMB(I,I)#1. PRIM0330
      SYMB(I+1,I)#0. PRIM0340
3000 SYMB(I+5,I)#0. PRIM0350
      TAPER#.375 PRIM0360
      THETA#0.0 PRIM0370
      VIEW#0.0 PRIM0380
      XLNG(I)#30.0 PRIM0390
      XLNG(2)#11.0 PRIM0400
      XO(1)#15.0 PRIM0410
      XO(2)#5.5 PRIM0420
      RETURN PRIM0430
      END PRIM0440
*LIST8
*LABEL
      SUBROUTINE PROJ(D,DP,X,XO,VIEW,I1,I2,I3)
C      ***** 3D CARTESIAN TO 2D PLOTTER COORDINATES *****
      DIMENSION D(3,129),DP(2,129),X(3),XO(3) PROJ0010
      T3#VIEW-X(3) PROJ0020
      DO 145 I#I1,I2,I3 PROJ0030
      T1#D(1,I)+X(1) PROJ0040
      T2#D(2,I)+X(2) PROJ0050
      IF(VIEW)135,135,120 PROJ0060
120  T4#VIEW/(T3-D(3,I)) PROJ0070
      T1#T1*T4 PROJ0080
      T2#T2*T4 PROJ0090
135  DP(1,I)#T1+XO(1) PROJ0100
145  DP(2,I)#T2+XO(2) PROJ0110
      RETURN PROJ0120
      END PROJ0130
*LIST8
*LABEL

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C SUBROUTINE RADIAL(ND)                               RAD0010
C ***** GENERATE ELLIPSE FROM TWO CONJUGATE VECTORS *****  RAD0020
C ***** ORTHONORMAL VECTORS PRODUCE 8-128 SPOKED CIRCLE *****  RAD0030
C ***** ND DENOTES NUMBER OF SUBDIVISIONS (1 TO 5) *****  RAD0040
C DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)  RAD0050
C DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)  RAD0060
C DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3)  RAD0070
C DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  RAD0080
C DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  RAD0090
C DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)  RAD0100
C DIMENSION XLNG(3),XO(3),XT(3)                      RAD0110
C COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  RAD0120
C COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD  RAD0130
C COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1  RAD0140
C COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2  RAD0150
C COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                  RAD0160
C DO 115 J#1,3                                      RAD0170
C T1#DA(J,1)                                         RAD0180
C D(J,1)#T1                                         RAD0190
C D(J,129)#T1                                       RAD0200
C D(J,65)#-T1                                       RAD0210
C T1#DA(J,2)                                         RAD0220
C D(J,33)#T1                                         RAD0230
C 115 D(J,97)#-T1                                     RAD0240
C DO 135 K#1,ND                                      RAD0250
C T1#CONT(K)                                         RAD0260
C KDEL#2***(6-K)                                     RAD0270
C KDEL1#KDEL+1                                       RAD0280
C KDEL2#KDEL/2                                       RAD0290
C DO 135 L#KDEL1,65,KDEL                         RAD0300
C J#L-KDEL                                         RAD0310
C M#L-KDEL2                                         RAD0320
C DO 135 N#1,3                                      RAD0330
C T2#(D(N,L)+D(N,J))#T1                           RAD0340
C D(N,M)#T2                                         RAD0350
C 135 D(N,M+64)#-T2                                RAD0360
C RETURN                                              RAD0370
C END                                                 RAD0380
*LIST8
*LABEL
SUBROUTINE SEARCH                                     SEAR0010
DIMENSION NW(6),DX(3),S(2,200),U(3),V(3),W(2,4),WW(2,3),X(4),Y(3)  SEAR0020
DIMENSION Z(3)                                         SEAR0030
DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)  SEAR0040
DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)  SEAR0050
DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3)  SEAR0060
DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  SEAR0070
DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)  SEAR0080
DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)  SEAR0090
DIMENSION XLNG(3),XO(3),XT(3)                      SEAR0100
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  SEAR0110
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD  SEAR0120
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1  SEAR0130
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2  SEAR0140
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                  SEAR0150
EQUIVALENCE(NW(1),LL),(NW(2),LU),(NW(3),ML)          SEAR0160
EQUIVALENCE(NW(4),MU),(NW(5),NL),(NW(6),NU)          SEAR0170
C **** OBTAIN PROBLEM PARAMETERS ****                 SEAR0180
WRITE OUTPUT TAPE NOUT,20                            SEAR0190
20 FORMAT(IHD 9X,82H   FROM ATOMS      TO ATOMS      WITH RADIUS OR  SEAR0200
I, IF A BOX, WITH SEMIDIMENSIONS /1IX,46HCODE (MIN MAX) (MIN MSEAR0210
2AX)           7X,IHA8X,IHB8X,IHC)                   SEAR0220
IF(AIN(1)-10000.)100,100,101                      SEAR0230
100 ITCM1#AIN(1)                                     SEAR0240
SYITOM#55501.                                         SEAR0250
GO TO 103                                           SEAR0260
101 ITCM1#AIN(1)/100000.                           SEAR0270
SYITOM#MODF(AIN(1),100000.)                       SEAR0280
102 IF(AIN(2)-10000.)103,103,104                  SEAR0290
103 ITCM2#AIN(2)                                     SEAR0300

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      GO TO 105                               SEAR0310
104 ITCM2#AIN(2)/100000.                   SEAR0320
105 ITARI#AIN(3)                           SEAR0330
      IF(ITARI)108,108,110                 SEAR0340
108 ITARI#1                                SEAR0350
110 ITAR2#AIN(4)                           SEAR0360
      DMAX#AIN(5)                           SEAR0370
      IF(DMAX)115,115,120                 SEAR0380
115 DMAX#4.                                SEAR0390
      AIN(5)#DMAX                          SEAR0400
120 DMX#DMAX=DMAX                         SEAR0410
      TEM#.01                             SEAR0420
      KFUN#NJ=100+XMODF(NJ2,10)           SEAR0430
      K#NJ*100+NJ2                         SEAR0440
      10#SYITCM                           SEAR0450
121 FORMAT(IH010X,2I3,2I5,I7,I5,18X,3F9.3/IH ) SEAR0460
      WRITE OUTPUT TAPE NOUT,121,K,ITOM1,I0,ITOM2,ITARI,ITAR2,(AIN(J),J#SEAR0470
      15,7)                                 SEAR0480
124 FORMAT(IH 15X,2I5,I8,I5,2F9.3)          SEAR0490
      IF(NCD)130,130,125                 SEAR0500
125 WRITE OUTPUT TAPE NOUT,124,((KDI(J,I),J#I,4),(CD(J,I),J#I,2)),I#I,SEAR0510
      (NCD)                                SEAR0520
130 DO 135 J#I,4                           SEAR0530
      W(I,J)#99.                          SEAR0540
135 W(2,J)#-99.                           SEAR0550
      DO 155 I#ITARI,ITAR2               SEAR0560
      TI#FLOATF(I)*100000.                SEAR0570
      CALL ATOM(TI,X)                     SEAR0580
      IF(NG)140,145,140                 SEAR0590
140 CALL ERPN(TI,KFUN)                    SEAR0600
      GO TO 600                           SEAR0610
145 X(4)#X(1)-X(2)                      SEAR0620
      DO 155 J#I,4                           SEAR0630
      TEM#X(J)                           SEAR0640
      IF(W(2,J)-TEM)148,150,150          SEAR0650
148 W(2,J)#TEM                           SEAR0660
150 IF(TEM-W(I,J))152,155,155          SEAR0670
152 W(I,J)#TEM                           SEAR0680
155 CONTINUE                            SEAR0690
      IF(KFUN-403)165,160,600            SEAR0700
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES MODEL BOX *****
160 DO 162 J#I,3                           SEAR0710
      DX(J)#0.                           SEAR0720
      DO 162 I#I,3                           SEAR0730
162 DX(J)#DX(J)+ABSF(REFV(J,I)*AIN(I+4)) SEAR0740
      GO TO 170                           SEAR0750
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES DMAX SPHERE *****
165 TI#1.-A(4)*A(4)-A(5)*A(5)-A(6)*A(6)+2.*A(4)*A(5)*A(6) SEAR0760
      DO 168 J#I,3                           SEAR0770
168 DX(J)#SQRTF((1.-A(J+3)**2/TI)*DMAX/A(J)) SEAR0780
C     ***** START SEARCH AROUND REFERENCE ATOMS *****
170 DO 500 ITOM#ITOM1,ITOM2               SEAR0790
      TI#FLOATF(ITOM)=100000.+SYITOM        SEAR0800
      CALL ATOM(TI,Y)                      SEAR0810
      IF(NG)171,172,171                 SEAR0820
171 CALL ERPN(TI,KFUN)                    SEAR0830
      GO TO 500                           SEAR0840
C     ***** K#SYMMETRY EQUIVALENT POSITION *****
172 NUM#0                                SEAR0850
173 DO 400 K#I,NSYM                      SEAR0860
C     ***** SUBTRACT SYMMETRY TRANSLATION FROM REF ATOM *****
      DO 175 J#I,3                           SEAR0870
175 U(J)#Y(J)-TS(J,K)                   SEAR0880
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****
      DO 185 J#I,3                           SEAR0890
      DO 185 L#I,2                           SEAR0900
      WW(L,J)#0.0                          SEAR0910
      DO 185 I#I,3                           SEAR0920
      TEM#FS(I,J,K)                      SEAR0930
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****
      DO 185 J#I,3                           SEAR0940
      DO 185 L#I,2                           SEAR0950
      WW(L,J)#0.0                          SEAR0960
      DO 185 I#I,3                           SEAR0970
      TEM#FS(I,J,K)                      SEAR0980
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****
      DO 185 J#I,3                           SEAR0990
      DO 185 L#I,2                           SEAR1000
      WW(L,J)#0.0                          SEAR1000

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      IF(ITEM)177,185,179          SEARI010
177 N#XMODF(L,2)+1           SEARI020
      GO TO 183                 SEARI030
179 N#L                         SEARI040
183 WW(L,J)#WW(L,J)+W(N,I)*TEM SEARI050
185 CONTINUE                     SEARI060
C     ***** CHECK FOR MIXED INDEX TRANSFORMATION *****
C     DO 215 J#1,2               SEARI070
      TEM#FS(I,J,K)             SEARI080
      IF(ITEM+FS(2,J,K))215,201,215 SEARI090
201 IF(ITEM)203,215,207         SEARI100
203 WW(I,J)#W(2,4)*TEM        SEARI120
      WW(2,J)#W(1,4)*TEM        SEARI130
      GO TO 215                 SEARI140
207 WW(I,J)#W(1,4)*TEM        SEARI150
      WW(2,J)#W(2,4)*TEM        SEARI160
215 CCNTINUE                   SEARI170
C     ***** MOVE 4 CELLS AWAY THEN MOVE BACK UNTIL PARALLELEPIPED AROUNDSEARI180
C     REF ATOM AND BOX AROUND TRANSFORMED ASYM UNIT INTERSECT ***** SEARI190
C     N#D
C     DO 235 J#1,3               SEARI200
      DO 225 I#1,2               SEARI210
      #N+1
      TT#(U(J)-WW(I,J))*FLOATF(I*2-3)-DX(J)   SEARI220
      TEM#5.0
221 TEM#TEM-I.0                SEARI230
      IF(ITEM+TT)225,225,221           SEARI240
225 NW(N)#TEM*FLOATF(I*2-3)+5.  SEARI250
C     ***** IF NO POSSIBILITY OF A HIT, GO TO NEXT SYMMETRY OPER ***** SEARI260
      IF(NW(N)-NW(N-1))400,235,235           SEARI270
235 CCNTINUE                   SEARI280
C     ***** L CELL TRANSLATIONS IN X *****
C     DO 395 L#LL,LU              SEARI290
      V(1)#U(1)+FLOATF(L-5)           SEARI300
C     ***** M CELL TRANSLATIONS IN Y *****
C     DO 395 M#ML,MU              SEARI310
      V(2)#U(2)+FLOATF(M-5)           SEARI320
C     ***** N CELL TRANSLATIONS IN Z *****
C     DO 395 NN#NL,NU              SEARI330
      V(3)#U(3)+FLOATF(NN-5)           SEARI340
C     ***** I # TARGET ATOM *****
C     DO 395 I#ITARI,ITAR2          SEARI350
      DO 250 J#1,3               SEARI360
      TEM#0.0
      DO 245 II#I,3               SEARI370
245 TEM#TEM+FS(II,J,K)*P(II,I)  SEARI380
C     ***** SEE IF WITHIN PARALLELEPIPED*****
      TEM#TEM-V(J)                SEARI390
      IF(DX(J)-TEM)395,395,250           SEARI400
250 X(J)#TEM                  SEARI410
      IF(KFUN-403)255,252,255           SEARI420
C     ***** SEE IF WITHIN MODEL BOX *****
252 CALL VM(X,AAREV,VI(2))       SEARI430
      DO 253 J#2,4               SEARI440
      IF(AIN(J+3)-ABSF(VI(J)))395,253,253 SEARI450
253 CCNTINUE                   SEARI460
      GO TO 277                 SEARI470
C     ***** SEE IF WITHIN SPHERE *****
255 DSQ#VMV(X,AA,X)             SEARI480
      IF(DMX-DSQ)395,256,256           SEARI490
256 IF(DSQ-.0001)258,260,260           SEARI500
258 IF(KFUN-402)395,260,395           SEARI510
C     ***** SELECT VECTORS ACCORDING TO CODES IF ANY *****
260 TEM#SQRTF(DSQ)             SEARI520
      IF(NCD)277,277,268           SEARI530
268 DO 275 J#1,NCD             SEARI540
269 IF(ITOM-KD(I,J))275,270,270           SEARI550
270 IF(KD(2,J)-ITOM)275,271,271           SEARI560
271 IF(I-KD(3,J))    275,272,272           SEARI570
272 IF(KD(4,J)-I)    275,273,273           SEARI580

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273 IF(TEM-CD(I,J)) 275,274,274 SEAR1710
274 IF(CD(2,J)-TEM) 275,277,277 SEAR1720
275 CONTINUE SEAR1730
276 GO TO 395 SEAR1740
277 VI(I) # 100000.*FLOATF(I)+FLOATF((I+L+100-M+10-NN)*100+K) SEAR1750
278 IF(KFUN=402)278,325,325 SEAR1760
C **** DETERMINE CORRECT POSITION IN SORTED VECTOR TABLE **** SEAR1770
279 IF(NUM)317,317,279 SEAR1780
280 DO 315 II#I,NUM SEAR1790
281 TT#S(2,II)-TEM SEAR1800
282 IF(ABSF(TT)-0.0001)297,297,281 SEAR1810
283 IF(200-NUM)287,287,289 SEAR1820
284 NUM#199 SEAR1830
285 IJ#NUM SEAR1840
286 DO 295 J#II,NUM SEAR1850
287 S(1,IJ+1)#S(1,IJ) SEAR1860
288 S(2,IJ+1)#S(2,IJ) SEAR1870
289 IJ#IJ-1 SEAR1880
290 GO TO 319 SEAR1890
C ***** CHECK FOR DUPLICATE VECTORS IF DISTANCES ARE EQUAL *****
291 CALL ATOM(S(1,II),Z) SEAR1900
292 DO 305 J#1,3 SEAR1910
293 IF(ABSF(X(J)+Y(J)-Z(J))-0.0001)305,305,315 SEAR1920
294 CONTINUE SEAR1930
295 GO TO 395 SEAR1940
296 315 CCNTINUE SEAR1950
297 IF(200-NUM)395,395,317 SEAR1960
C **** STORE THE RESULT IN VECTOR TABLE *****
298 317 II#NUM+1 SEAR1970
299 319 NUM#NUM+1 SEAR1980
300 S(1,II)#VI(I) SEAR1990
301 S(2,II)#TEM SEAR2000
302 GO TO 395 SEAR2010
C **** STORE RESULT IN ATOMS TABLE *****
303 325 DO 330 J#1,3 SEAR2020
304 330 VI(J+1)#X(J)+Y(J) SEAR2030
305 CALL STORE SEAR2040
306 395 CCNTINUE SEAR2050
307 400 CONTINUE SEAR2060
C **** PRINT OUT DISTANCES *****
308 421 FORMAT(IH1DX,2DHVECTORS FROM ATOM (I3,IH,I5,IH)6X,8HTO ATOMSI4, SEAR2070
309 18H THROUGHI4) SEAR2080
310 422 IO#SYITCM SEAR2090
311 WRITE OUTPUT TAPE NOUT,421,ITOM,IO,ITARI,ITAR2 SEAR2100
312 IF(NUM)500,500,423 SEAR2110
313 423 DO 435 I#I,NUM SEAR2120
314 T2#S(1,I) SEAR2130
315 II#T2/100000. SEAR2140
316 I2#T2-FLOATF(II)*100000. SEAR2150
317 CALL ATOM(T2,Z) SEAR2160
318 IF(I-1)432,432,434 SEAR2170
319 427 FORMAT(IH 13X,2(A6,IX),39X,IH(I3,IH,I5,IH)3F7.4,7X,3HD #F6.3) SEAR2180
320 428 FORMAT(IH 13X,2(A6,IX),2(3H (I3,IH,I5,IH)3F7.4,3X)4X,3HD #F6.3) SEAR2190
321 429 WRITE OUTPUT TAPE NOUT,429,CHEM(ITOM),CHEM(II),ITCM,IO,(Y(J),J#I,3 SEAR2200
322 1),II,I2,(Z(J),J#I,3),S(2,I) SEAR2210
323 GO TO 435 SEAR2220
324 434 WRITE OUTPUT TAPE NOUT,427,CHEM(ITOM),CHEM(II),II,I2,(Z(J),J#I,3), SEAR2230
325 IS(2,I) SEAR2240
326 435 CCNTINUE SEAR2250
C **** CALCULATE ANGLES ABOUT REF ATOM IF CODE IS 102 *****
327 437 IF(NJ2=21500,451,451 SEAR2260
328 441 FORMAT(IH1DX,18HANGLES AROUND ATOMIS) SEAR2270
329 451 WRITE OUTPUT TAPE NOUT,441,ITOM SEAR2280
330 L#NUM-1 SEAR2290
331 IF(L)500,500,457 SEAR2300
332 457 DO 465 I#I,L SEAR2310
333 T2#S(1,I) SEAR2320
334 T3#S(2,I) SEAR2330

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I1#T2/100000.                               SEAR2410
I2#T2-FLOATF(I1)*100000.                   SEAR2420
CALL ATOM(T2,X)                           SEAR2430
CALL DIFV(X,Y,U)                          SEAR2440
CALL MV(AA,U,V2)                          SEAR2450
M#I+1                                     SEAR2460
DO 465 J#M,NUM                           SEAR2470
T4#S(1,J)                                 SEAR2480
J1#T4/100000.                            SEAR2490
J2#T4-FLOATF(J1)*100000.                  SEAR2500
CALL ATOM(T4,Z)                           SEAR2510
CALL DIFV(Z,Y,V)                          SEAR2520
F#ARCCOS(VV(V,V2)/(T3*S(2,J)))          SEAR2530
460 FORMAT(IH 13X,3(A6,IX),7X,3(2H (I3,IH,I5,IH)),3IX,F6.2) SEAR2540
465 WRITE OUTPUT TAPE NOUT,460,CHEM(I1),CHEM(ITOM),CHEM(J1),I1,I2,ITOMSEAR2550
   J,I0,J1,J2,F                           SEAR2560
495 CONTINUE                                SEAR2570
500 CCNTINUE                               SEAR2580
600 RETURN                                  SEAR2590
END                                       SEAR2600

*LIST8
*LABEL
      SUBROUTINE SPARE(NJ)                  SPAR0010
      COMMON NG                           SPAR0020
      NG#9                             SPAR0030
      RETURN                           SPAR0040
      END                               SPAR0050

*LIST8
*LABEL
      SUBROUTINE STORE                  STOR0010
C      ***** STORE IN OR REMOVE FROM ATOMS ARRAY *****
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) STOR0020
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130) STOR0030
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) STOR0040
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) STOR0050
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) STOR0060
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3) STOR0070
      DIMENSION XLNG(3),X0(3),XT(3)           STOR0080
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D STOR0090
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD STOR0100
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI STOR0110
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2 STOR0120
      COMMON V3,V4,V5,V6,WRKV,XLNG,X0,XT           STOR0130
      IF(LATM)481,481,450                      STOR0140
450 IF(500-LATM)455,455,460                  STOR0150
455 IF(NJ2-I0)490,490,460                  STOR0160
460 LATM#LATM                               STOR0170
C      ***** CHECK FOR POSITIONAL DUPLICATION *****
      DO 480 K#1,L                         STOR0180
      DO 465 J#2,4                         STOR0190
      IF(ABSF(VI(J)-ATOMS(I,K))-0.001)465,465,480 STOR0200
465 CONTINUE                                STOR0210
      IF(NJ2-I0)490,490,470                  STOR0220
C      ***** ATOM REMOVAL BY TABLE PUSHDOWN *****
470 LATM#LATM-1                           STOR0230
      DO 475 I#K,LATM                      STOR0240
      DO 475 J#1,4                         STOR0250
475 ATCMS(J,I)#ATOMS(J,I+1)                STOR0260
      GO TO 490                           STOR0270
480 CCNTINUE                               STOR0280
481 IF(NJ2-I0)482,490,490                  STOR0290
C      ***** STORE ATOM *****
482 IF(499-LATM)490,483,485                STOR0300
483 NG#16                                    STOR0310
      CALL ERPNT (VI(),400)                 STOR0320
485 LATM#LATM+1                           STOR0330
      DO 486 J#1,4                         STOR0340
486 ATCMS(J,LATM)#VI(J)                  STOR0350
490 RETURN                                  STOR0360
      END                                     STOR0370
                                         STOR0380
                                         STOR0390
                                         STOR0400
                                         STOR0410

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*LIST8
*LABEL
    SUBROUTINE TMM(X,Y,Z)
    ***** TRANPOSE(TRANPOSE(X)*Y)*Z *****
C     ***** X,Y,Z ARE 3X3 MATRICES *****
C     DIMENSION X(3,3),Y(3,3),Z(3,3)
C     DO 115 I#1,3
C     DO 115 K#1,3
115 Z(K,I)*X(I,K)+X(2,I)*Y(2,K)+X(3,I)*Y(3,K)
    RETURN
    END

*LIST8
*LABEL
    SUBROUTINE UNIT(X,Z,ITYPE)
    DIMENSION X(3),Y(3),Z(3)
    DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
    DIMENSION ATCMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)
    DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3)
    DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
    DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)
    DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
    DIMENSION XLNG(3),X0(3),XT(3)
    COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
    COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD
    COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL
    COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
    COMMON V3,V4,V5,V6,WRKV,XLNG,X0,XT
    Y(1)*X(1)
    Y(2)*X(2)
    Y(3)*X(3)
    IF(ITYPE)125,125,105
105 TI#SQRTF(Y(1)*Y(1)+Y(2)*Y(2)+Y(3)*Y(3))
    GO TO 145
125 TI#SQRTF(Y(1)*(Y(1)*AA(1,1)+Y(2)*(AA(1,2)+AA(2,1))+Y(3)*(AA(1,3)+AA(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2))+Y(3)*Y(3)*AA(3,3)))
    1A(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2))+Y(3)*Y(3)*AA(3,3))
    2,3))
145 IF(TI)155,155,175
155 NG#5
    GO TO 300
175 Z(1)*Y(1)/TI
    Z(2)*Y(2)/TI
    Z(3)*Y(3)/TI
300 RETURN
    END

*LIST8
*LABEL
    SUBROUTINE VM(X,Y,Z)
    TRANSPOSED VECTOR TIMES MATRIX
C     Z(3)*X(3)*Y(3,3)
    DIMENSION X(3),Y(3,3),Z(3)
    DO 115 J#1,3
    Z(J)*0.0
    DO 115 I#1,3
115 Z(J)*Z(J)+X(I)*Y(I,J)
    RETURN
    END

*LIST8
*LABEL
    FUNCTION VMV(X1,Q,X2)
    TRANSPOSED VECTOR * MATRIX * VECTOR
C     VMV#X1(3)*Q(3,3)*X2(3)      TO EVALUATE QUADRATIC OR BILINEAR FORM
    DIMENSION X1(3),Q(3,3),X2(3)
    TI#0.
    DO 10 J#1,3
10 TI#TI+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))
    VMV#TI
    RETURN
    END

*LIST8
*LABEL

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FUNCTION VV(X,Y) VV 0010
C TRANSPOSED VECTOR * VECTOR VV 0020
C VV#X(3)*Y(3) VV 0030
DIMENSION X(3),Y(3) VV 0040
VV#X(1)*Y(1)+X(2)*Y(2)+X(3)*Y(3) VV 0050
RETURN VV 0060
END VV 0070
*LIST8
*LABEL
SUBROUTINE XYZ(QA,X,ITYPE) XYZ 0010
C ***** ITYPE .GT.0 CART. COORD. FROM ATOM CODE WORD ***** XYZ 0020
C ***** XABSF(ITYPE) .LE.2 FOR WORKING SYSTEM ***** XYZ 0030
C ***** XABSF(ITYPE) .GT.2 FOR REFERENCE SYSTEM ***** XYZ 0040
C ***** ITYPE .LE.0 USES TRICLINIC COORD. XT ***** XYZ 0050
DIMENSION X(3) XYZ 0060
DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140) XYZ 0070
DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)XYZ 0080
DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3)XYZ 0090
DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)XYZ 0100
DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48) XYZ 0110
DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)XYZ 0120
DIMENSION XLNG(3),XO(3),XT(3) XYZ 0130
COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D XYZ 0140
COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATP,LTNO,NATOM,NCD XYZ 0150
COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI XYZ 0160
COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2 XYZ 0170
COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT XYZ 0180
IT#XABSF(ITYPE)-2 XYZ 0190
NG#NG XYZ 0200
NG#J XYZ 0210
IF(ITYPE)10,10,5 XYZ 0220
5 CALL ATCM(QA,XT) XYZ 0230
IF(NG)30,10,30 XYZ 0240
10 TI#0. XYZ 0250
DO 15 J#1,3 XYZ 0260
T2#XT(J)-ORGN(J) XYZ 0270
V1(J)#T2 XYZ 0280
15 TI#TI+ABSF(T2) XYZ 0290
IF(TI-.0001)20,20,40 XYZ 0300
20 NG#NG1 XYZ 0310
30 DO 35 J#1,3 XYZ 0320
35 X(J)#0. XYZ 0330
GO TO 300 XYZ 0340
40 IF(IT)45,45,60 XYZ 0350
C ***** RELATIVE TO WORKING SYSTEM ***** XYZ 0360
45 DO 55 I#1,3 XYZ 0370
TI#0. XYZ 0380
DO 50 J#1,3 XYZ 0390
50 TI#TI+V1(J)*AAWRK(J,I) XYZ 0400
55 X(I)#TI#SCALI XYZ 0410
GO TO 300 XYZ 0420
C ***** RELATIVE TO REFERENCE SYSTEM ***** XYZ 0430
60 DO 70 I#1,3 XYZ 0440
TI#0. XYZ 0450
DO 65 J#1,3 XYZ 0460
65 TI#TI+V1(J)*AAREV(J,I) XYZ 0470
70 X(I)#TI#SCALI XYZ 0480
300 RETURN XYZ 0490
END XYZ 0500

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