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OR TEP-II: A FORTRAN Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations

Carroll K. Johnson

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CHEMISTRY DIVISION

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

Carroll K. Johnson

Revised February 1976

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

Carroll K. Johnson

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 most recent version of the program, OR TEP-II, has a hidden-line-elimination feature to omit those portions of atoms or bonds behind other atoms or bonds.

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 the scientific literature, 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 add further detail, often 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, require a minimum of input, and be easy to modify. (4) The computation time should be minimized. Memory size limitation was not of the considerations; hence the program requires at least 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. Busing[2] 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-II FORTRAN IV listing for the IBM 360.

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.

---

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

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

[3] W. 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	D max (A)	–	–
Dist. + ang.	0 or 2	102	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Princ. axes	–	103	–	–	–	–	–	–	–
Dist. single convolute	–	105	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Dist. reiterate convolute	–	106	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Plotter control									
Initialize	–	201	–	–	–	–	–	–	–
Advance and term.	–	202	X(IN)	Y(IN)	–	–	–	–	–
Initialize CRT	–	203	XORG	YORG	IZORG				
Change CRT intensity	–	204	IZ-IZORG						
Plot boundary									
Dimensions	–	301	X(IN)	Y(IN)	VIEW(IN)	BRDR(IN)	–	–	–
Title rotation	–	302	THETA(°)	–	–	–	–	–	–
Retrace displace	–	303	X(IN)	–	–	–	–	–	–
Atoms list									
Run add	–	401	FROM (1)	(–) TO (1)	FROM (2)	(–) TO (2)	FROM (3)	(–) TO (3)	. . .
Run subtract	–	411	FROM (1)	(–) TO (1)	FROM (2)	(–) TO (2)	FROM (3)	(–) TO (3)	. . .
Sphere add	0 or 2	402	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)	–	–
Sphere subtract	0 or 2	412	ORG 1	ORG 2	TAR 1	TAR 2	D max (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)
Triclinic box add	–	404	ORG 1	ORG 2	TAR 1	TAR 2	A/2	B/2	C/2
Triclinic box subtract	–	414	ORG 1	ORG 2	TAR 1	TAR 2	A/2	B/2	C/2
Convolute add	–	405	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Convolute subtract	–	415	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Reiterate convolute add	–	406	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Reiterate convolute subt.	–	416	ORG 1	ORG 2	TAR 1	TAR 2	D max (A)		
Zero atoms list	–	410	–	–	–	–	–	–	–
Cartesian system									
Definition	–	501	ORGN	V1A	V1B	V2A	V2B	–	–
Rotate reference	–	502	Axis No.	Rotate (°)	Axis No.	Rotate (°)	. . .	. . .	. . .
Rotate working	–	503	Axis No.	Rotate (°)	–	–	–	–	–
Translate working	–	504	ΔX (IN)	ΔY (IN)	ΔZ (IN)	–	–	–	–
Origin at centroid	–	505	–	–	–	–	–	–	–
Inertial axis system and origin at centroid	–	506	–	–	–	–	–	–	–
Store overlap data (Also see 822, 821)	0 or 2	511	0 –1 OVMRGN (IN)						

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)	ANR (1)	ANR (2)	–	–	–
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)	ANR (1)	ANR (2)			
As above except no	0 or 1	711	(same as 701)						
printed output of	0 or 1	712	(same as 701)						
individual coordinates	0 or 1	713	(same as 701)						
	0 or 1	714	(same as 701)						
	0 or 1	715	(same as 705)						
Bonds									
Explicit (cont.)	1 or 2	801	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	. . .
Implicit fancy (Format No. 2 trailer card)	2	802	–	–	–	–	–	–	–
Implicit line (Format No. 2 trailer card)	2	803	–	–	–	–	–	–	–
As above except	–	811	(same as 801)						
no printed output	2	812	(same as 802)						
	2	813	(same as 803)						
Bond overlap explicit	1 or 2	821	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	. . .
Bond overlap implicit	2	822	–	–	–	–	–	–	–
Labels									
Chem. Symb.	–	901	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Reg. titles. Format No. 3 title card	3	902	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Proj. Vect. title Format No. 3 title card	3	903	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Vector title Format No. 3 title card	3	913	ATOM-1	ATOM-2	–	–	HGT (IN)	PAR-OFF	PER-OFF

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Proj. bond label									
(1 dec. place)	–	904	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(2 dec. places)	–	905	(same as 904)						
(3 dec. places)	–	906	(same as 905)						
Bond label									
(1 dec. place)	–	914	ATOM-1	ATOM-2	–	–	HGT (IN)	PAR-OFF	PER-OFF
(2 dec. places)	–	915	(same as 914)						
(3 dec. places)	–	916	(same as 914)						
Centered symb. (pen up)	1	908	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
(pen down)	1	909	(same as 908)						
(Format No. 1 trailer card)		–	SYMB#	–	–	–	–	–	–
Saved sequence	–								
Start	–	1101	–	–	–	–	–	–	–
Stop	–	1102	–	–	–	–	–	–	–
Execute	–	1103	–	–	–	–	–	–	–
Terminate job	–	–1	–	–	–	–	–	–	–
New job follows (from title card on)	–	–2	–	–	–	–	–	–	–

[a]I.P. and I.S. signifies increment position and increment scale.
[b]PAR-OFF signifies parallel offset (in.).
[c]PER-OFF signifies perpendicular offset (in.).

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.

The major portions of the hidden line segments of atoms and bonds that are partially or totally behind other atoms and bonds may be omitted by using the overlap-elimination features of OR TEP-II. However, there are often areas where additional manual touch-up is needed. This can be accomplished by erasing or "whiting out" the remaining unwanted line segments. Even with stereo views, the features 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 parts of Sect. 2, and the individual instructions are described in detail in Sect. 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 triclinic box of enclosure can be described with a 404 instruction (see 3.3.5.4) 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.

A new instruction 511 in the OR TEP-II version of the program was added to store information needed for the overlap correction. This instruction is used before the 700 and 800 series instructions.

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) is 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° 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 cubane[4] (C_4H_4) 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 $R\bar{3}$. 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

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

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

The equivalent positions of space group[6] $R\bar{3}$ 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 zero[7] 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 3.2.3)

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

---

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

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

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

[7] Unfortunately, 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 3.2.4.1): FORMAT (A6, 3X, 5F9.6, F9.0)

Thermal parameters (see 3.2.4.2): FORMAT (11, 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 A 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 next to 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 3.3.1.4) 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 Sect. 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 A about the two carbons C1 and C2, one would use the following instruction. (The notation is explained in Sect. 3.3.2.)

Card No.

(19) 101 155501 2 1 4 3.61

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

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 1.5-in. margin to give a total working area of 9 by 9 in. A 30-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 30 1.5

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 A should be adequate to isolate a single molecule.

Card No.

(24) 402 555501 5 (a) 1 4 (b) 3.2 (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 A.

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

To scale and position the subject for projection onto the drawing board and to utilize all available space, we will use the 604 instruction, which 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.

(27) 604 0 0 0 1.54

This completes the composition of the illustration.

The stereoscopic rotation for the left eye can be done at this point. We will use a rotation of 2.7° about the *Y* axis (axis 2) for the left-eye view. Later in the program, we will make a −2.7° rotation about the same axis for the right-eye view to give a total interocular angle of 5.4°.

(28) 503 2 2.7

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

Card No.

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.

(29)		1101								

The 511 instruction stores the information needed for the overlap hidden-line correction (i.e., as projected boundary ellipses for each atom in the ATOMS list and a quadrangle approximation for each bond). The bonds are specified with a format No. 2 trailer card identical to that used in the 812 instruction described below.

(30)	2	511			0					
(31)		0	1	4	1	4	4	0.9	1.6	.04

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 draw the carbon atoms (ANR = 1,2), 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)	1	715		4	0	1	0	.2	.6	.7
(33)		0		0	0	1	2			

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.

Since the hydrogen atoms (ANR = 3, 4) 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.

(34)	1	712		0	0	0	0	.2	.35	.4
(35)		0		0	0	3	4			

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).

Card No.

(36) 2 812

(37) 0 $\underbrace{1 \quad 4}_{(a)}$ $\underbrace{1 \quad 4}_{(b)}$ $\underbrace{4}_{(c)}$ $\underbrace{.9 \quad 1.6}_{(d)}$ $\underbrace{.04}_{(e)}$

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 A, which will cover all covalent bond distances, and

(*e*) the bond radius, is 0.04 A.

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.

(38)	906	155504	155503	0	0	.15	0	–.4
(39)	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.

(40)	3	902	555501	0	0	1.	.25	0	0

(41) CUBANE

The saved sequence can now be terminated.

(42) 1102

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

(43) 202 9

The stereo rotation of –2.7° 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.)

(44) 503 2 –2.7

Card No.

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.

(45) 1103

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

(46) 202 20

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

(47) 202 0

Finally we terminate the job and exit from the program.

(48) −1

2.4.4 Stereoscopic Illustration of the Examples. – Figure 2.1 shows the stereoscopic pair exactly as it was plotted by a mechanical CalComp system, except for photographic reduction. Figure 2.2 shows one-half of the same illustration at a larger scale. These drawings have not been retouched.

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.

Figure 2.3 is an example of a figure without photographic reduction drawn by a CalComp plotter which has 0.005 in. step-size resolution. Another representation of the same structure is shown in Fig. 6.19.

The input data and OR TEP instructions for Fig. 2.3 are listed in 2.4.5.2. The user should examine this example carefully since several useful techniques are illustrated.

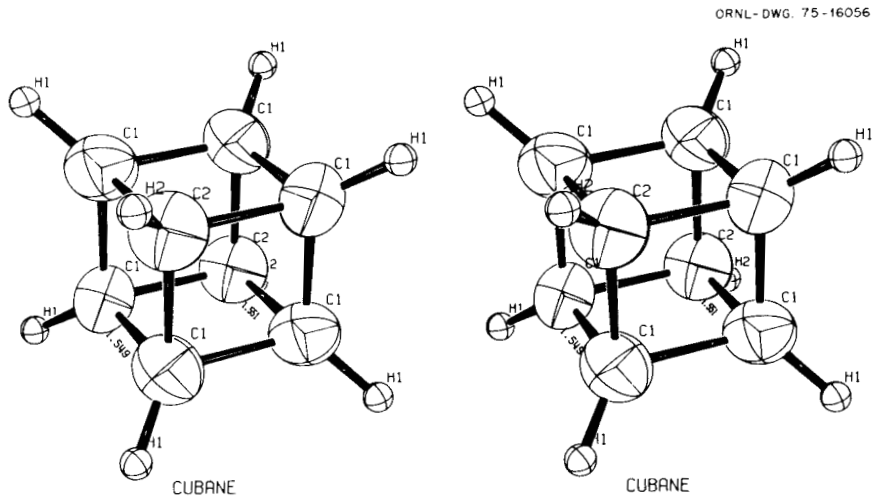

Fig. 2.1. The Sample Figure Cubane Reduced for Stereoscopic Viewing.

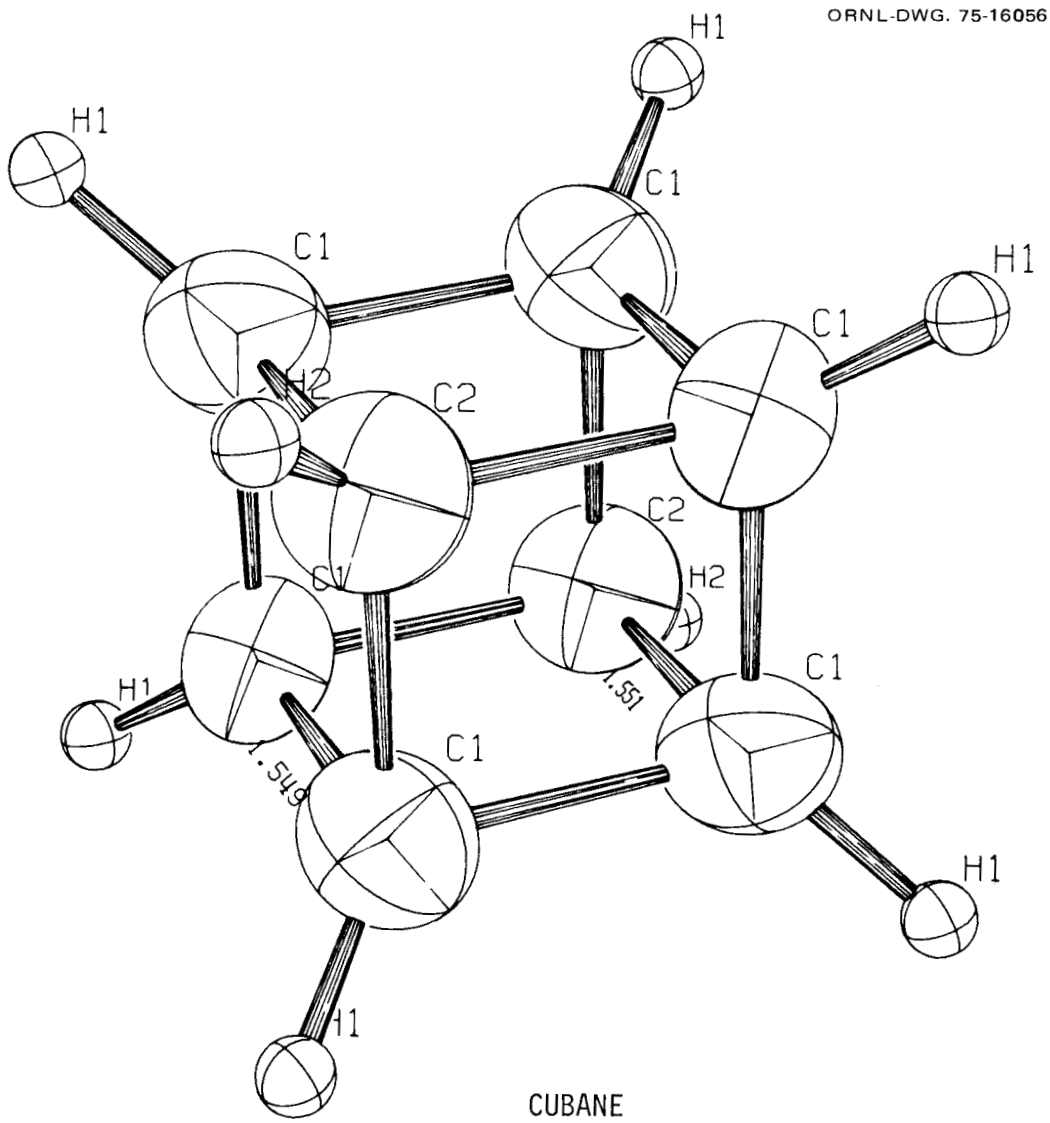

Fig. 2.2. The Sample Figure Cubane at 82% of Original Scale.

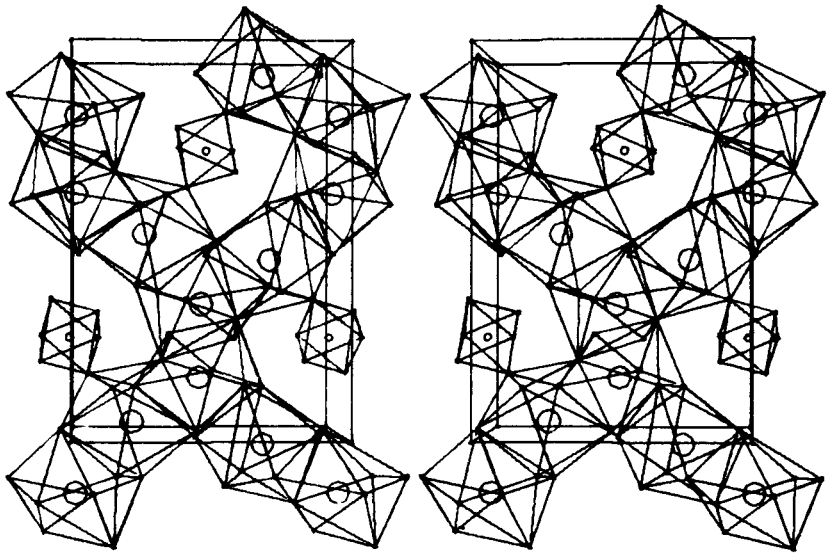

Fig. 2.3 Polyhedra Representation of Potassium Perxenate 9-Hydrate.

2.4.5 Listing of Sample Input and Output. – *2.4.5.1 Listing of Input Cards for Cubane.* –

```
 CUBANE  E.B.FLEISCHER    1964  J.A.C.S.  86,3889                          EXAM  10
     5.34      5.34      5.34     72.26     72.26     72.26                 EXAM  20
               0  1  0  0                0  0  1  0                0  0  0  1EXAM  30
               0  0  0  1                0  1  0  0                0  0  1  0EXAM  40
               0  0  1  0                0  0  0  1                0  1  0  0EXAM  50
               0 -1  0  0                0  0 -1  0                0  0  0 -1EXAM  60
               0  0  0 -1                0 -1  0  0                0  0 -1  0EXAM  70
1              0  0 -1  0                0  0  0 -1                0 -1  0  0EXAM  80
  C1                            -.18711   .19519   .10706         0         EXAM  90
   .04100   .04250   .04500   -.00420  -.01420  -.00510         0         EXAM 100
  C2                             .11546   .11546   .11546         0         EXAM 110
   .04630   .04680   .04680   -.01430  -.01430  -.01430         0         EXAM 120
  H1                            -.32460   .34680   .18480         0         EXAM 130
      .10                                                         7         EXAM 140
  H2                             .21000   .21000   .21000         0         EXAM 150
      .10                                                         7         EXAM 160
 ORGN                                 0        0        0         0         EXAM 170
1                                                                 0         EXAM 180
  3   101   1555C1        2        1        4     3.61                     EXAM 190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****         EXAM 200
  3   102   1555C1        2        1        4      1.8                     EXAM 210
***** FIND COVALENT BONDS AND BOND ANGLES ARCUND CARBONS *****             EXAM 220
  3   201                                                                 EXAM 230
***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****     EXAM 240
  3   301      11.      11.      30.      1.5                             EXAM 250
***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****     EXAM 260
  3   303                                                                 EXAM 270
***** ELIMINATE ALL RETRACING *****                                        EXAM 280
  3   402   555501        5        1        4      3.2                     EXAM 290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****      EXAM 300
  3   501   555501   255501   155501   255501   155502                  0EXAM 310
***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****EXAM 320
  3   502        2      25.        1      28.                             EXAM 330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****         EXAM 340
  3   604        0        0        0     1.54                             EXAM 350
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **EXAM 360
  3   503        2      2.7                                               EXAM 370
```

```
***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****          EXAM 380
  3  1101                                                                EXAM 390
***** START SAVE SEQUENCE *****                                          EXAM 400
  2   511        0                                                       EXAM 410
  3        1  4  1  4  4   0.9   1.6   .04                               EXAM 420
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULTEXAM 430
  1   715        4        0        1        0      .20      .60      .70EXAM 440
  3                                 1        2                          EXAM 450
***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****             EXAM 460
  1   712                                          .20      .35      .40EXAM 470
  3                                 3        4                          EXAM 480
***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****              EXAM 490
  2   812                                                                EXAM 500
  3        1  4  1  4  4   0.9   1.6   .04                               EXAM 510
***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A EXAM 520
  3   906   155504   155503        0        0      .15        0      -.4EXAM 530
***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****   EXAM 540
  3   916   255504   155505        0        0      .15        0      -.4EXAM 550
***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****EXAM 560
  3   902   555501        0        0      1.0      .25        0        0EXAM 570
                                CUBANE                                   EXAM 580
  3  1102                                                                EXAM 590
***** END OF SAVE SEQUENCE *****                                         EXAM 600
  3   202       9.                                                       EXAM 610
***** ADVANCE PLOTTER 9 INCHES ALONG X *****                             EXAM 620
  3   503        2     -2.7                                              EXAM 630
***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****   EXAM 640
  3  1103                                                                EXAM 650
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****                 EXAM 660
  3   202      20.                                                       EXAM 670
***** ADVANCE PLOTTER 20 INCHES *****                                    EXAM 680
  3   202                                                                EXAM 690
***** ADD DUMMY PLOT TO MAGNETIC TAPE *****                              EXAM 700
      -1                                                                 EXAM 710
```

2.4.5.2 Listing of Input Cards for Potassium Perxenate 9-Hydrate. –

```
 POTASSIUM PERXENATE 9-HYDRATE/A.ZALKIN ET AL /(1964) JACS 86,3569       EXAM0010
    9.049   10.924   15.606      90.       90.       90.                 EXAM0020
            .0  1  0  0            .0  0  1  0            .0  0  0  1EXAM0030
            .0 -1  0  0            .0  0 -1  0            .5  0  0  1EXAM0040
            .0 -1  0  0            .5  0  1  0            .0  0  0  1EXAM0050
1           .0  1  0  0            .5  0 -1  0            .5  0  0  1EXAM0060
  XE                              .249      .988      .250              EXAM0070
     .10                                                   7            EXAM0080
  K1                              .628      .987      .339              EXAM0090
     .30                                                   7            EXAM0100
  K2                              .846      .238      .958              EXAM0110
     .30                                                   7            EXAM0120
  K3                              .307      .227      .026              EXAM0130
     .30                                                   7            EXAM0140
  K4                              .877      .989      .139              EXAM0150
     .30                                                   7            EXAM0160
  C1                              .403      .101      .251              EXAM0170
     .20                                                   7            EXAM0180
  C2                              .094      .878      .253              EXAM0190
     .20                                                   7            EXAM0200
  C3                              .138      .096      .316              EXAM0210
     .20                                                   7            EXAM0220
  O4                              .176      .058      .151              EXAM0230
     .20                                                   7            EXAM0240
  C5                              .323      .918      .351              EXAM0250
     .20                                                   7            EXAM0260
```

```
  O6                                .360     .881     .188                    EXAM0270
     .20                                                          7           EXAM0280
  W1                                .654     .839     .190                    EXAM0290
     .20                                                          7           EXAM0300
  W2                                .850     .136     .297                    EXAM0310
     .20                                                          7           EXAM0320
  W3                                .873     .829     .369                    EXAM0330
     .20                                                          7           EXAM0340
  W4                                .692     .046     .506                    EXAM0350
     .20                                                          7           EXAM0360
  W5                                .997     .243     .111                    EXAM0370
     .20                                                          7           EXAM0380
  W6                                .967     .980     .972                    EXAM0390
     .20                                                          7           EXAM0400
  W7                                .376     .470     .002                    EXAM0410
     .20                                                          7           EXAM0420
  W8                                .493     .262     .886                    EXAM0430
     .20                                                          7           EXAM0440
  W9                                .606     .150     .124                    EXAM0450
     .20                                                          7           EXAM0460
 ORGN                               .250     .500     .400                    EXAM0470
     .10                                                          7           EXAM0480
                                    .000     .000     .000                    EXAM0490
1    .03                                                          7           EXAM0500
  3   102   155501   555501         1        20      3.55                    EXAM0510
***** DISTANCES,ANGLES AND EDGES OF XE AND K COORDINATION POLYHEDRA ****EXAM0520
  3   201                                                                    EXAM0530
***** INITIALIZE CALCOMP PLOT PACKAGE *****                                  EXAM0540
  3   301        10        11        12      3.85                           EXAM0550
***** 10-2*3.85 # 2.3 IN. DIAMETER PICTURES,12 IN. AWAY,DIRECT STEREO VUEXAM0560
  3   401  225501 -226601                                                    EXAM0570
***** STORE UNIT CELL CORNERS FOR CELL OUTLINE *****                         EXAM0580
  3   404        21        21         1         5       .13       .52      .57EXAM0590
***** STORE CENTRAL ATOMS OF POLYHEDRA ****                                  EXAM0600
  3   405         1         5         1        20      3.52                EXAM0610
***** CONVOLUTE SPHERE OF ENCLOSURE WITH EACH CENTRAL ATOM *****             EXAM0620
  3   501  215501  215501  215601  215501  215601                          1EXAM0630
***** B AXIS HORIZONTAL, C AXIS VERTICAL, VIEWED ALONG -A AXIS *****         EXAM0640
  3   604                                                                    EXAM0650
***** AUTOMATIC SCALE AND POSITION *****                                     EXAM0660
  3   503         2         3                                                EXAM0670
***** STEREO ROTATION FOR LEFT EYE VIEW *****                                EXAM0680
  3  1101                                                                    EXAM0690
***** START SAVED SEQUENCE *****                                             EXAM0700
  1   714                                                                    EXAM0710
  3                                   1         5                            EXAM0720
***** DRAW METAL ATOMS SELECTIVELY *****                                     EXAM0730
  2   813                                                                    EXAM0740
  2       22 22 22 22   1   9.0  11.0   .01                                  EXAM0750
  2       22 22 22 22   1  15.0  16.0   .01                                  EXAM0760
  2        6 11  6 11   3   2.5   2.8   .04    -1      1   1.8   1.9        EXAM0770
  2        6 19  6 19   1   2.6   4.4   .02    -2      2   2.6   3.1        EXAM0780
  2       10 20 10 20   1   2.6   4.7   .02    -3      3   2.7  3.52        EXAM0790
  2        9 20  9 20   1   2.6  4.58   .02    -4      4   2.7   3.3        EXAM0800
  3        7 20  7 20   1   2.6   4.6   .02    -5      5   2.7   3.2        EXAM0810
***** DRAW POLYHEDRA AND CELL OUTLINE *****                                  EXAM0820
  3  1102                                                                    EXAM0830
***** END SAVED SEQUENCE *****                                               EXAM0840
  3   202       2.4                                                          EXAM0850
***** ADVANCE PLOTTER FOR RIGHT EYE VIEW *****                               EXAM0860
  3   503         2        -3                                                EXAM0870
***** STEREO ROTATION FOR RIGHT EYE VIEW *****                               EXAM0880
  3  1103                                                                    EXAM0890
***** REPEAT SAVED SEQUENCE                                                  EXAM0900
  3   202        10                                                          EXAM0910
***** ADVANCE PLOTTER 10 IN. *****                                           EXAM0920
  3   202                                                                    EXAM0930
***** ADD DUMMY PLOT  ( STOP CALCOMP ON PLOT NO. 3 ) *****                   EXAM0940
       -1                                                                    EXAM0950
```

2.4.5.3 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
5.339999	5.339999	5.339999	72.260	72.260	72.260
		COSINE	0.30469871	0.30469871	0.30469871

RECIPROCAL CELL PARAMETERS

A*	B*	C*	ALPHA*	BETA*	GAMMA*
0.202207	0.202207	0.202207	103.506	103.506	103.506
		COSINE	-0.23353952	-0.23353940	-0.23353940

SYMMETRY TRANSFORMATIONS

NO.		TRANSFORMED X		TRANSFORMED Y		TRANSFORMED Z	
1	0.0	1. X 0. Y 0. Z	0.0	0. X 1. Y 0. Z	0.0	0. X 0. Y 1. Z	
2	0.0	0. X 0. Y 1. Z	0.0	1. X 0. Y 0. Z	0.0	0. X 1. Y 0. Z	
3	0.0	0. X 1. Y 0. Z	0.0	0. X 0. Y 1. Z	0.0	1. X 0. Y 0. Z	
4	0.0	-1. X 0. Y 0. Z	0.0	0. X -1. Y 0. Z	0.0	0. X 0. Y -1. Z	
5	0.0	0. X 0. Y -1. Z	0.0	-1. X 0. Y 0. Z	0.0	0. X -1. Y 0. Z	
6	0.0	0. X -1. Y 0. Z	0.0	0. X 0. Y -1. Z	0.0	-1. X 0. Y 0. Z	

NO.	ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23	TYPE
1	C1	-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	H1	-0.324600	0.346800	0.184800	0.100000	0.0	0.0	0.0	0.0	0.0	7.
4	H2	0.210000	0.210000	0.210000	0.100000	0.0	0.0	0.0	0.0	0.0	7.
5	ORGN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.

NO.	ATOM	X	Y	Z	RMSD 1	RMSD 2	RMSD 3
1	C1	-0.187110	0.195190	0.107060	0.204899	0.239856	0.255794
2	C2	0.115460	0.115460	0.115460	0.205704	0.247732	0.247732
3	H1	-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	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                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR          Y VECTOR          Z VECTOR
   0.1872659E 00  -0.5990840E-01  -0.4722326E-01          0.5339996E 01   0.9536743E-06   0.9536743E-06
   0.0             0.1966153E 00  -0.4722328E-01          0.1627090E 01   0.5086076E 01   0.9536743E-06
   0.0             0.0             0.2022068E 00          0.1627090E 01   0.1187799E 01   0.4945430E 01

((((( INSTRUCTION  101 )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.3610000E 01  0.0            0.0

***** FIND ALL NEIGHBOR ATOMS AROUND C1 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   255501   1   4                        3.610    0.0      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                                          (  1,55505)-0.1071 0.1871-0.1952        D = 1.549
     C1      C1                                          (  1,55506)-0.1952-0.1071 0.1871        D = 1.549
     C1      C2                                          (  2,55501) 0.1155 0.1155 0.1155        D = 1.552
     C1      C1                                          (  1,55502) 0.1071-0.1871 0.1952        D = 2.183
     C1      C1                                          (  1,55503) 0.1952 0.1071-0.1871        D = 2.183
     C1      C2                                          (  2,55504)-0.1155-0.1155-0.1155        D = 2.202
     C1      H1                                          (  3,55506)-0.3468-0.1848 0.3246        D = 2.282
     C1      H1                                          (  3,55505)-0.1848 0.3246-0.3468        D = 2.306
     C1      H2                                          (  4,55501) 0.2100 0.2100 0.2100        D = 2.376
     C1      C1                                          (  1,55504) 0.1871-0.1952-0.1071        D = 2.677
     C1      H1                                          (  3,55502) 0.1848-0.3246 0.3468        D = 3.052
     C1      H1                                          (  3,55503) 0.3468 0.1848-0.3246        D = 3.069
     C1      H2                                          (  4,45501)-0.7900 0.2100 0.2100        D = 3.077
     C1      H2                                          (  4,56504)-0.2100 0.7900-0.2100        D = 3.096
     C1      H2                                          (  4,55504)-0.2100-0.2100-0.2100        D = 3.175
     C1      H1                                          (  3,55605)-0.1848 0.3246 0.6532        D = 3.200
     C1      H1                                          (  3,45603)-0.6532 0.1848 0.6754        D = 3.284
     C1      H1                                          (  3,46504)-0.6754 0.6532-0.1848        D = 3.388
     C1      C2                                          (  2,36504)-0.1155 0.8845-0.1155        D = 3.609

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                                          (  1,55501)-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
     C2      C1                                          (  1,55504) 0.1871-0.1952-0.1071        D = 2.202
     C2      C1                                          (  1,55505)-0.1071 0.1871-0.1952        D = 2.202
     C2      C1                                          (  1,55506)-0.1952-0.1071 0.1871        D = 2.202
     C2      H1                                          (  3,55501)-0.3246 0.3468 0.1848        D = 2.273
     C2      H1                                          (  3,55502) 0.1848-0.3246 0.3468        D = 2.273
     C2      H1                                          (  3,55503) 0.3468 0.1848-0.3246        D = 2.273
     C2      C2                                          (  2,35504)-0.1155-0.1155-0.1155        D = 2.710
     C2      H1                                          (  3,55504) 0.3246-0.3468-0.1848        D = 3.091
     C2      H1                                          (  3,55505)-0.1848 0.3246-0.3468        D = 3.091
     C2      H1                                          (  3,35506)-0.3468-0.1848 0.3246        D = 3.091
     C2      H1                                          (  3,56504) 0.3246 0.6532-0.1848        D = 3.181
     C2      H1                                          (  3,55605)-0.1848 0.3246 0.6532        D = 3.181
     C2      H1                                          (  3,65506) 0.6532-0.1848 0.3246        D = 3.181
     C2      C1                                          (  1,36504) 0.1871 0.8048-0.1071        D = 3.609
     C2      C1                                          (  1,55605)-0.1071 0.1871 0.8048        D = 3.609
     C2      C1                                          (  1,65506) 0.8048-0.1071 0.1871        D = 3.609
```

```
((((( INSTRUCTION  102 )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.1799999E 01  0.0            0.0

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

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

102  155501   255501   1   4                        1.800    0.0      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                                            (  1,55505)-0.1071 0.1871-0.1952        D = 1.549
     C1     C1                                            (  1,55506)-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) (  1,55505)            D = 2.282        A =124.69
     H1     C1     C1          (  3,55501) (  1,55501) (  1,55506)            D = 2.306        A =127.16
     H1     C1     C2          (  3,55501) (  1,55501) (  2,55501)            D = 2.273        A =123.52
     C1     C1     C1          (  1,55505) (  1,55501) (  1,55506)            D = 2.183        A = 89.60
     C1     C1     C2          (  1,55505) (  1,55501) (  2,55501)            D = 2.202        A = 90.48
     C1     C1     C2          (  1,55506) (  1,55501) (  2,55501)            D = 2.202        A = 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                                            (  1,55501)-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)            D = 2.376        A =125.66
     H2     C2     C1          (  4,55501) (  2,55501) (  1,55502)            D = 2.376        A =125.66
     H2     C2     C1          (  4,55501) (  2,55501) (  1,55503)            D = 2.376        A =125.66
     C1     C2     C1          (  1,55501) (  2,55501) (  1,55502)            D = 2.183        A = 89.44
     C1     C2     C1          (  1,55501) (  2,55501) (  1,55503)            D = 2.183        A = 89.44
     C1     C2     C1          (  1,55502) (  2,55501) (  1,55503)            D = 2.183        A = 89.44

((((( INSTRUCTION  201 )))))
 0.0            0.0            0.0            0.0            0.0            0.0            0.0

***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****

((((( INSTRUCTION  301 )))))
 0.1100000E 02  0.1100000E 02  0.3000000E 02  0.1500000E 01  0.0            0.0            0.0

***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****

PLOT LIMITS 11.00 BY 11.00 IN.  INCLUDING  1.50  IN. MARGIN
VIEW DISTANCE 30.000 INCHES
```

```
((((( INSTRUCTION  303 )))))
      0.0          0.0          0.0          0.0          0.0          0.0          0.0

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

      RETRACE DISPLACEMENT = 0.0    INCH

((((( INSTRUCTION  402 )))))
      0.5555010E 06  0.5000000E 01  0.1000000E 01  0.4000000E 01  0.3200000E 01  0.0          0.0

      ***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****

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

      402  555501   555501   1    4                       3.200    0.0      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          0.0

      ***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****

      ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.      0.0          0.0          0.0

      ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES              POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
        -0.1950173E 00  -0.5332431E-01  0.3517698E-02          -0.5161572E 01  0.2128973E 00  0.1352190E 01
         0.5138889E-01   0.4031152E-02  0.1955263E 00          -0.2760968E 00  0.1350079E 01  0.5159129E 01
        -0.5414121E-02   0.1954785E 00 -0.5144400E-01          -0.1402325E 01  0.5145890E 01  0.2624693E 00

((((( INSTRUCTION  502 )))))
      0.2000000E 01  0.2500000E 02  0.1000000E 01  0.2800000E 02  0.0          0.0          0.0

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

      ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.      0.0          0.0          0.0

      ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES              POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
        -0.1752591E 00  -0.8727211E-01  0.5055124E-01          -0.4106512E 01 -0.1411451E 01  0.3108037E 01
         0.1292071E 00  -0.6943828E-01  0.1391812E 00           0.1930112E 01 -0.1057861E 01  0.4865296E 01
        -0.2664803E-01   0.1934117E 00  0.5262519E-01          -0.1160014E 01  0.4153644E 01  0.3149157E 01

((((( INSTRUCTION  604 )))))
      0.0          0.0          0.0          0.1540000E 01  0.0          0.0          0.0

      ***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **

      ORIGIN POINT IN PLOTTER COORD.(  5.35 ,  5.75 ) IN.
      OVERALL SCALE = 1.960 INCH/ANGSTROM ELLIPSOID SCALE = 1.540
      VIEW DISTANCE 30.000 INCHES
```

```
((((( INSTRUCTION  503 )))))
 0.2000000E 01  0.2700000E 01  0.0            0.0            0.0            0.0            0.0

***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR        Y VECTOR        Z VECTOR
  -0.1726831E 00  -0.8727211E-01   0.5875095E-01          -0.3955544E 01  -0.1411451E 01   0.3298029E 01
   0.1356199E 00  -0.6943828E-01   0.1329401E 00           0.2157155E 01  -0.1057861E 01   0.4768971E 01
  -0.2413946E-01   0.1934117E 00   0.5382206E-01          -0.1010380E 01   0.4153644E 01   0.3200305E 01

((((( INSTRUCTION 1101 )))))
 0.0            0.0            0.0            0.0            0.0            0.0            0.0

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

((((( INSTRUCTION  511 )))))
 0.0            0.0            0.0            0.0            0.0            0.0            0.0
   1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT

OVERLAP MARGIN IS 0.042 INCH
CONTENTS OF SORTED ATOMS ARRAY
       455504.   255504.   355504.   355506.   155504.   155506.   355505.   155505.   355502.   155502.
       155503.   155501.   355503.   355501.   255501.   455501.

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   0.040   0.0     0.0     0.0     0.0       0.
FAULT NG = 14   455504.   800


BOND OVERLAP ARRAY CONTAINS  19 BONDS (MAXIMUM IS 599)
ATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE IN SORTED ATOMS ARRAY
         2005.     2006.     2008.     3005.     4006.     5010.     5011.     6010.     6012.     7008.
         8011.     8012.     9010.    10015.    11013.    11015.    12014.    12015.    15016.

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES              POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR        Y VECTOR        Z VECTOR
  -0.1752591E 00  -0.8727211E-01   0.5055124E-01          -0.4106512E 01  -0.1411451E 01   0.3108037E 01
   0.1292071E 00  -0.6943828E-01   0.1391812E 00           0.1930112E 01  -0.1057861E 01   0.4865296E 01
  -0.2664803E-01   0.1934117E 00   0.5262519E-01          -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  715 )))))
 0.4000000E 01  0.0            0.1000000E 01  0.0            0.2000000E 00  0.6000000E 00  0.7000000E 00
 0.0            0.0            0.1000000E 01  0.2000000E 01  0.0            0.0            0.0

***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
```

```
((((( INSTRUCTION  712 )))))
      0.0            0.0            0.0            0.0            0.2000000E 00  0.3500000E 00  0.4000000E 00
      0.0            0.0            0.3000000E 01  0.4000000E 01  0.0            0.0            0.0

     ***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****

((((( INSTRUCTION  812 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0
        1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

     ***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A

     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   0.040   0.0     0.0     0.0     0.0       0.
     FAULT NG = 14    455504.    800


((((( INSTRUCTION  906 )))))
      0.1555040E 06  0.1555030E 06  0.0            0.0            0.1500000E 00  0.0            -0.4000000E 00

     ***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****

((((( INSTRUCTION  916 )))))
      0.2555040E 06  0.1555050E 06  0.0            0.0            0.1500000E 00  0.0            -0.4000000E 00

     ***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****

((((( INSTRUCTION  902 )))))
      0.5555010E 06  0.0            0.0            0.1000000E 01  0.2500000E 00  0.0            0.0

                                      CUBANE

((((( INSTRUCTION 1102 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

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

((((( INSTRUCTION  202 )))))
      0.9000000E 01  0.0            0.0            0.0            0.0            0.0            0.0

     ***** ADVANCE PLOTTER 9 INCHES ALONG X *****

((((( INSTRUCTION  503 )))))
      0.2000000E 01 -0.2700000E 01  0.0            0.0            0.0            0.0            0.0

     ***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****

     ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

     ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
          X VECTOR        Y VECTOR        Z VECTOR
       -0.1774457E 00  -0.8727211E-01   0.4223930E-01          -0.4248351E 01  -0.1411451E 01   0.2911142E 01
        0.1225073E 00  -0.6943828E-01   0.1451131E 00           0.1698782E 01  -0.1057861E 01   0.4950814E 01
       -0.2909743E-01   0.1934117E 00   0.5131147E-01          -0.1307071E 01   0.4153644E 01   0.3091016E 01
```

```
((((( INSTRUCTION 1103 )))))
 0.0          0.0          0.0          0.0          0.0          0.0          0.0

***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****

((((( INSTRUCTION  511 )))))
 0.0          0.0          0.0          0.0          0.0          0.0          0.0
   1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT

OVERLAP MARGIN IS 0.042 INCH

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

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   0.040   0.0     0.0     0.0     0.0       0.
FAULT NG = 14   455504.   800


BOND OVERLAP ARRAY CONTAINS  19 BONDS (MAXIMUM IS 599)
ATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE IN SORTED ATOMS ARRAY
         2005.     3005.     3006.     3010.     4006.     5009.     5011.     6009.     6012.     7010.
         8009.     9015.    10011.    10012.    11013.    11015.    12014.    12015.    15016.

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.       0.0            0.0            0.0

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR         Y VECTOR         Z VECTOR
  -0.1752591E 00  -0.8727211E-01   0.5055124E-01          -0.4106512E 01  -0.1411451E 01   0.3108037E 01
   0.1292071E 00  -0.6943828E-01   0.1391812E 00           0.1930112E 01  -0.1057861E 01   0.4865296E 01
  -0.2664803E-01   0.1934117E 00   0.5262519E-01          -0.1160014E 01   0.4153644E 01   0.3149157E 01

((((( INSTRUCTION  715 )))))
 0.4000000E 01  0.0            0.1000000E 01  0.0            0.2000000E 00  0.6000000E 00  0.7000000E 00
 0.0            0.0            0.1000000E 01  0.2000000E 01  0.0            0.0            0.0

***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
((((( INSTRUCTION  712 )))))
 0.0            0.0            0.0            0.0            0.2000000E 00  0.3500000E 00  0.4000000E 00
 0.0            0.0            0.3000000E 01  0.4000000E 01  0.0            0.0            0.0

***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****
```

```
((((( INSTRUCTION  812 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0
        1  4  1  4  4    0.90000    1.60000    0.04000    0.0        0.0        0.0        0.0        0.0

     ***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A

     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   0.040   0.0     0.0     0.0     0.0       0.
     FAULT NG = 14   455504.   800


((((( INSTRUCTION  906 )))))
      0.1555040E 06  0.1555030E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

     ***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****

((((( INSTRUCTION  916 )))))
      0.2555040E 06  0.1555050E 06  0.0            0.0            0.1500000E 00  0.0           -0.4000000E 00

     ***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ****

((((( INSTRUCTION  902 )))))
      0.5555010E 06  0.0            0.0            0.1000000E 01  0.2500000E 00  0.0            0.0

                                      CUBANE

((((( INSTRUCTION 1102 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

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

((((( INSTRUCTION  202 )))))
      0.2000000E 02  0.0            0.0            0.0            0.0            0.0            0.0

     ***** ADVANCE PLOTTER 20 INCHES *****

((((( INSTRUCTION  202 )))))
      0.0            0.0            0.0            0.0            0.0            0.0            0.0

     ***** ADD 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.

$$ADC = AN*10^5 + (TA + 5)*10^4 + (TB + 5)*10^3 + (TC + 5)*10^2 + SN,$$

where

AN = *ATOM NUMBER* ($0 \leqq AN \leqq NATOM \leqq 166$) = 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.).

TA,TB,TC = *crystal lattice translation digits* along cell edges **a**, **b**, and **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.

SN = *symmetry operator number* ($0 \leqq SN \leqq NSYM \leqq 48$) = 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 and is usually the first operator.

Example: An atom designation code of *3 475 02* refers to atom 3 moved through symmetry operation 2, then translated – 1 cell translation along **a**, +2 cell translations along **b**, and 0 cell translations along **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 × 9 × 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 **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, **a** translation TA; fourth, **b** translation TB; and last, **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 A to 2.4 A. 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 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:

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

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 17.0 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 α	α^* (deg)	cos α^*
37–45	β (deg)	cos β	β^* (deg)	cos β^*
46–54	γ (deg)	cos γ	γ^* (deg)	cos γ^*

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

3.2.3 Symmetry Cards (1 ≦ NSYM ≦ 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 operation[2] along the **c*** crystal axis

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

[2]The 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.

This 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[3]: 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

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

(*b*) Helix screw symmetry:

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

where

$\mathbf{T} = (T_1,\ T_2,\ T_3 + L/N)$ 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 $N = 18$; $M = 5$; $L = 0, 1, \ldots, 17$; $T_1, T_2, T_3 = 0$. The input atom list contains the contents of one residue.

3.2.4 Atom Parameter Cards (1 $\leq$ NATOM $\leq$ 166). – Two cards are required for each input atom. The first contains the chemical symbol and positional parameters, and the second contains temperature factor

[3]Only symmetry cards for *general* symmetry equivalent positions are permitted. Symmetry cards which explicitly designate special positions such as *X, X, X; X, X, Z; X,Y,*0; ¼,*Y*,0; and ¼,¾,0 *are not allowed.*

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 (°) 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 0,1,2,3,10	Type 4,5,8,9	Type 6		Type 7	
2–9	b_{11}	U_{11}	B	B	R	R
10–18	b_{22}	U_{22}	0	0	0	0
19–27	b_{33}	U_{33}	0	[VDC$_1$]	0	[VDC$_1$]
28–36	b_{12}	U_{12}	0		0	
37–45	b_{13}	U_{13}	0	[VDC$_2$]	0	[VDC$_2$]
46–54	b_{23}	U_{23}	0		0	
55–63	0,1,2,3,10	4,5,8,9	6 (or 0)	6 (or 0)	7	7

[4]W. 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 0,1,2,3,10, are defined as follows: The complete temperature factor is

$$(\text{Base})^{\{-D(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + c\, b_{12}hk + c\, b_{13}hl + c\, b_{23}kl)\}}$$

where in type 0: Base = e, $C = 2$, $D = 1$;

type 1: Base = e, $C = 1$, $D = 1$;

type 2: Base = 2, $C = 2$; $D = 1$;

type 3: Base = 2, $C = 1$, $D = 1$;

type 10: Base = e, $C = 2$, $D = 2\pi^2$.

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

$$\exp\left\{ -D\ (a_1^{*2}U_{11}h^2 + a_2^{*2}U_{22}k^2 + a_3^{*2}U_{33}l^2 + Ca_1^*a_2^*U_{12}hk + Ca_1^*a_3^*U_{13}hl + Ca_2^*a_3^*U_{23}kl)\right\} ,$$

where a_1^*, a_2^*, a_3^* are reciprocal cell dimensions and in types 4 and 8, $C = 2$; in types 5 and 9, $C = 1$; in types 4 and 5, $D = \frac{1}{4}$; in types 8 and 9, $D = 2\pi^2$. 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 arbitary orthogonal vectors by using the two vector designator codes VDC_1 and VDC_2; then the three new principal-axis vectors will be VDC_1, $(VDC_1 \times VDC_2)$, and $VDC_1 \times (VDC_1 \times VDC_2)$. This is strictly an artistic feature of no physical significance.

Type 7 allows the input of arbitrary spheres of radius $\overline{\mu} = R$ 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 $R = 0.1$ A.

A type 10 temperature-factor input card may be used to load Cartesian temperature factors having components in the standard Cartesian system (3.1.8). This feature complements the type 3 Cartesian positional parameter input system (3.2.4.1) and is useful for plotting mean-square displacements caused by internal molecular motions as calculated from spectroscopic normal-coordinate analyses.[5,6]

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

[5] C. K. Johnson, chap. 9 in *Thermal Neutron Diffraction*, ed by B. T. M. Willis, p. 149, Oxford University Press, London, 1970.

[6] R. R. Holmes and R. M. Deiters, *J. Chem. Phys.* **51**, 4043 (1969).

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 ten 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 101 402 102 412	Inertial axes 505/506	Bond plotting instructions 801/811/821	Bond plotting instructions 802/812/822	Bond plotting instructions 803/813	Negative No. in columns 43 to 48: 802/812/822	Negative No. in columns 43 to 48: 803/813
1–3	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead
4–9	–	–	–	–	–	–	–
10–12	ORG. ANR	ANR	–	ANR (A)	ANR (A)	ANR (A)	ANR (A)
13–15			–				
16–18	TAR. ANR	–	–	ANR (B)	ANR (B)	ANR (B)	ANR (B)
19–21		–	–				
22–24	–	–	Bond type	Bond type	–	Bond type	–
25–30	*D* min (A)	Weight	–	*D* min (A)	*D* min (A)	*D* min (A)	*D* min (A)
31–36	*D* max (A)	–	–	*D* max (A)	*D* max (A)	*D* max (A)	*D* max (A)
37–42	–	–	Bond radius (A)	Bond radius (A)	–	Bond radius (A)	–
43–48	–	–	Perspective label hgt. (in.)	Perspective label hgt. (in.)	–	ANR (P)	ANR (P)
49–54	–	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–		
55–60	–	–	Nonperspective label hgt. (in.)	Nonperspective label hgt. (in.)	–	D_p min (A)	D_p min (A)
61–66	–	–	Perpendicular displ. (in.)	Perpendicular displ. (in.)	–	D_p max (A)	D_p max (A)
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 designator run (see 3.1.3) of origin atoms (Org. ADR) and an atom number run of target atoms (Tar. ANR). The Org. ADR 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 A. The Org. ADR is designated (365502, 5) or (365502, 565502)[7] 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. ADR (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.*[8]

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 and interatomic distances for the edges opposite the angles are also calculated and printed for the stored vectors. There will be $n(n-1)/2$ angles for n vectors.

---

[7]For the origin sequence 355501, 455501, 555501, an Org. ADR 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. ADR is designated as ORG 1, ORG 2; and Tar. ANR is denoted by TAR 1, TAR 2. A minus sign preceeding the second member of the Org. ADR is not required.

[8]H. 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.

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 3.3.5.

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-ADR (atom designator run)
28–36, 37–45	Target ANR (atom number run)
46–54	D max (A)

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-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	103
10–18	Blank

3.3.2.3 Instructions 105 and 106, Convoluting Sphere of Enclosure and Reiterative Convoluting Sphere of Enclosure. – These instructions utilize the ATOMS table and can only be used after one or more atoms have been placed in the table by a 401, 402, 403, or 404 instruction. The contents of the table are returned to the condition of entry at the conclusion of instructions 105 and 106.

All atoms in the ATOMS table which have atom numbers within the origin atom number run (Org. ANR) of the instruction are used as origin points. Interatomic distances for all neighboring atoms (whether or not in the ATOMS table) are found out to the specified radius. Vector-search-code (VSC) cards may be used for screening if desired.

Instructions 105 and 106 are similar, except that instruction 106 keeps repeating the "convolution" process until no new atoms with atom numbers within the Org. ANR are found.

Instruction 106 is useful for molecular structures where the atoms in the input asymmetric unit do not form an intact molecule. In a case of this nature, it is advisable to place a single atom into the ATOMS table with a 401 instruction and let a 106 instruction find the molecule. Care must be taken to specify a D max which will enclose only bonded atoms. The 106 instruction should *not* be used for structures forming infinite chains.

Columns	
1–3	0 or 2 (look ahead)
4–9	105 or 106
10–18, 19–27	Origin ANR (atom number run)
28–36, 37–45	Target ANR (atom number run)
46–54	D max (A)

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 765 and 835 off-line magnetic tape plotting systems[9] are given here.

3.3.3.1 Instruction 201, Plot Package Initialization, Mechanical Plotter. – This instruction (or a 203 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. If the 201 (203) and 301 instructions are omitted, all calculations are carried out but no plotting is done.

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

[9]The 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. (This was true in 1965 and is still true in 1975.)

3.3.3.3 Control Instructions for CalComp Model 835 Cathode-Ray-Tube Plotter. – In order to plot interchangeably on the CRT and the mechanical CalComp plotters, an extended 200 series of instructions is necessary.

A 203 instruction initializes the CRT plotter and is used in place of the 201 instruction. In general, no other changes are needed except that the plotting area specified by the 301 instruction must not exceed 17 in. in *x* and 11 in. in *y*. (The 301 primer constants are set accordingly.)

Columns		
1–3	Blank	
4–9	203	
10–18	XORG	(new position of the origin of plotter coordinates relative to the lower left-hand corner of the normal CRT plotting area)
19–27	YORG	
28–36	IZORG	(beam intensity origin)

The entries for XORG, YORG, and IZORG are normally zero or blank.

The beam intensity, IZ, can be changed from its initialized value IZ = IZORG + 18 to any other value in the range 0 to 30 with a 204 instruction. The usable range of IZ is about 12 to 24 with the higher values producing darker lines.

Columns	
1–3	Blank
4–9	204
10–18	IZ – IZORG

The frame advance instruction 202 is interpreted differently for CRT usage; however, the same 202 instruction cards used for a mechanical plotter plot can also be used for a CRT plot. Any positive number in columns 10 to 18 of the 202 instruction (3.3.3.2) will add a block address (i.e., plot number) to the magnetic tape and will advance the film to a new frame. A value of zero in columns 10 to 18 will add a block address but will not advance the film to a new frame, and a negative value will terminate the output magnetic tape file. It is not normally necessary to use the negative value option since the termination is taken care of automatically when the -1 instruction is executed if a 201 instruction was not executed after the 203 initialization instruction; however, if the mechanical plotter is to be used during the same job, the negative value option allows the CRT to be terminated properly before initialization of the mechanical plotter.

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 series), the center points of the atoms are prevented from falling in the margin; but the atom represen-

tation, 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)	17.
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. Retracing should not be used with a CRT plotting device.

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.

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 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	As described above
.	
.	
.	
64–72	

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 designator 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 ADR (see 3.3.2.1)
19–27	
28–36	Target ANR (see 3.3.2.1)
37–45	
46–54	$a/2$ (A)
55–63	$b/2$ (A)
64–72	$c/2$ (A)

3.3.5.4 Instructions 404 and 414, Triclinic Box of Enclosure Add and Triclinic Box of Enclosure Eliminate. – These instructions are similar to instructions 403 and 413, except that the triclinic box of enclosure is bounded by planes parallel to the principal planes of the crystal lattice. The semidimensions $a/2$, $b/2$, $c/2$ refer to fractional (triclinic) coordinates. To specify the contents of the conventional unit cell, one would use $a/2 = b/2 = c/2 = .5$, and the Org. ADR would refer to a point in the input atom list at 1/2, 1/2, 1/2.

3.3.5.5 Instructions 405, 406, 415, 416; Convoluting Sphere of Enclosure Add, Reiterative Convoluting Sphere of Enclosure Add, Convoluting Sphere of Enclosure Eliminate, and Reiterative Convoluting Sphere of Enclosure Eliminate. – These instructions are used in the same manner as instructions 105 and 106 (see 3.3.2.3). Their function is to add atoms to or eliminate atoms from the ATOMS table. A valid origin atom must be placed in the ATOMS list with a 401, 402, 403, or 404 instruction before the present instructions are used. All atoms in the ATOMS table which have atom numbers within the origin atom number run (Org. ANR) of the instruction are used as origin points of convolution.

An important use for the 405 instruction is to complete the coordination shells around metal atoms without having to describe any of the atoms individually. Another use might be to obtain a cluster of atoms out to the *n*th neighbor when only the distance to the first neighbor is known. This can be accomplished by using *n* consecutive 405 instructions with D max slightly more than the first neighbor distance.

Instruction 406 is useful for describing molecular compounds when an unfortunate choice of atoms for the input asymmetric unit does not allow the molecule to be described by a run. D max must be chosen judiciously so that the search does not cross molecular boundaries.

The input format is identical to that described in 3.3.2.3, with the appropriate instruction number in columns 4–9.

3.3.5.6 Option for Examining E-Map Results. – Stereoscopic drawings are useful for the rapid screening of *E* maps when direct methods are used for solving crystal structures. First the interpolated positions of the largest peaks in the Fourier synthesis *E* map are punched on cards directly by a Fourier program. Then OR TEP starts at a given peak (usually the largest) and does a reiterative-sphere-of-enclosure-add instruction (406) to isolate a molecule if one is present. In order to terminate the convolution procedure when extraneous "bridging peaks" link the molecules, a modification was added to the 406 instruction which allows an atom (in any of its equivalent positions) to be entered in the ATOMS list only once. To invoke this feature, a type 1 continuation card (3.3.1.2) with a 1 in column 18 is added to the 406 instruction. The 406 instruction operates normally if the continuation card is omitted (3.3.5.5).

3.3.5.7 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 noncollinear vectors, and OR TEP provides the two following separate techniques for performing this operation, using vector cross products of the two vectors **u** and **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	Origin (ADC)	000000
19–27	Vector $\mathbf{u}$ (VDC)	155501
28–36		165501
37–45	Vector $\mathbf{v}$ (VDC)	155501
46–54		156501
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.

Columns	
1–3	–
4–9	503
10–18	1,2,3
19–27	ω°

3.3.6.4 Optimal Parameters for Stereoscopic Drawings. – Figure 3.1 shows a geometrical construction which may be used to derive the parameters used in making stereoscopic drawings.[10,11] The empirical parameters in common usage [(*a*) 30-in. view distance, (*b*) 5° to 6° stereo rotation, and

[10] J. T. Rule, *J. Opt. Soc. Am.* **28**, 313 (1938).

[11] B. G. Saunders, *Appl. Opt.* **7**, 1499 (1968).

(c) a photographic reduction to achieve 2.2 to 2.4 in. separation of equivalent points] produce quite satisfactory results with a slightly exaggerated impression of depth. Theoretically, the best stereoscopic fidelity is obtained by translation of the origin rather than by stereo rotation of the object;[11] however, the comparison of results given in Fig. 3.2 shows that the differences are indeed minor and nearly impossible to detect. Stereo by translation of origin is achieved with instruction 504, which may be used in place of the 503 instruction; however, the 504 instructions should not be used when the ellipsoids have internal structure because the octants selected for shading may not be the same on both stereo views.

Columns

1–3	Blank
4–9	504
10–18	Translation of origin along x axis of reference system (in.)
19–27	Translation of origin along y axis of reference system (in.)
28–36	Translation of origin along z axis of reference system (in.)

For the geometrical conditions depicted in Fig. 3.1, the stereo-rotation instructions for the left and right eyes,

503 2 2.45

and

503 2 –2.45 ,

are replaced by the stereo translation instructions

504 –1.28 0 0

and

504 2.56 0 0 ,

respectively. If additional drawings are to be made, the origin first should be returned to its original position with the instruction

504 –1.28 0 0 ,

in order to prevent confusion.

3.3.6.5 Instruction 505, Origin at Centroid. – This instruction finds the first moment (i.e., centroid or center of gravity) of the atoms in the ATOMS list and makes this point the ORIGIN of the reference and working coordinate systems. A weighting scheme and screening may be applied to the atoms by using format No. 2 trailer cards (see Table 3.1). If no trailer cards are used, all atom positions are entered with unit weights.

3.3.6.6 Instruction 506, Origin at Centroid and Inertial Axis Coordinate System. – The calculation described for instruction 505 is performed; then the second moment matrix about the centroid is calculated, and the reference and working coordinate systems are set up along the principal axes of this matrix. This principal axis system of coordinates is along the inertial axis of the configuration of atoms in the ATOMS list. The x axis is along the long axis of the configuration (i.e., the minimum axis of inertia) and the z axis is along the short axis of the configuration (i.e. the maximal axis of inertia). The overlap

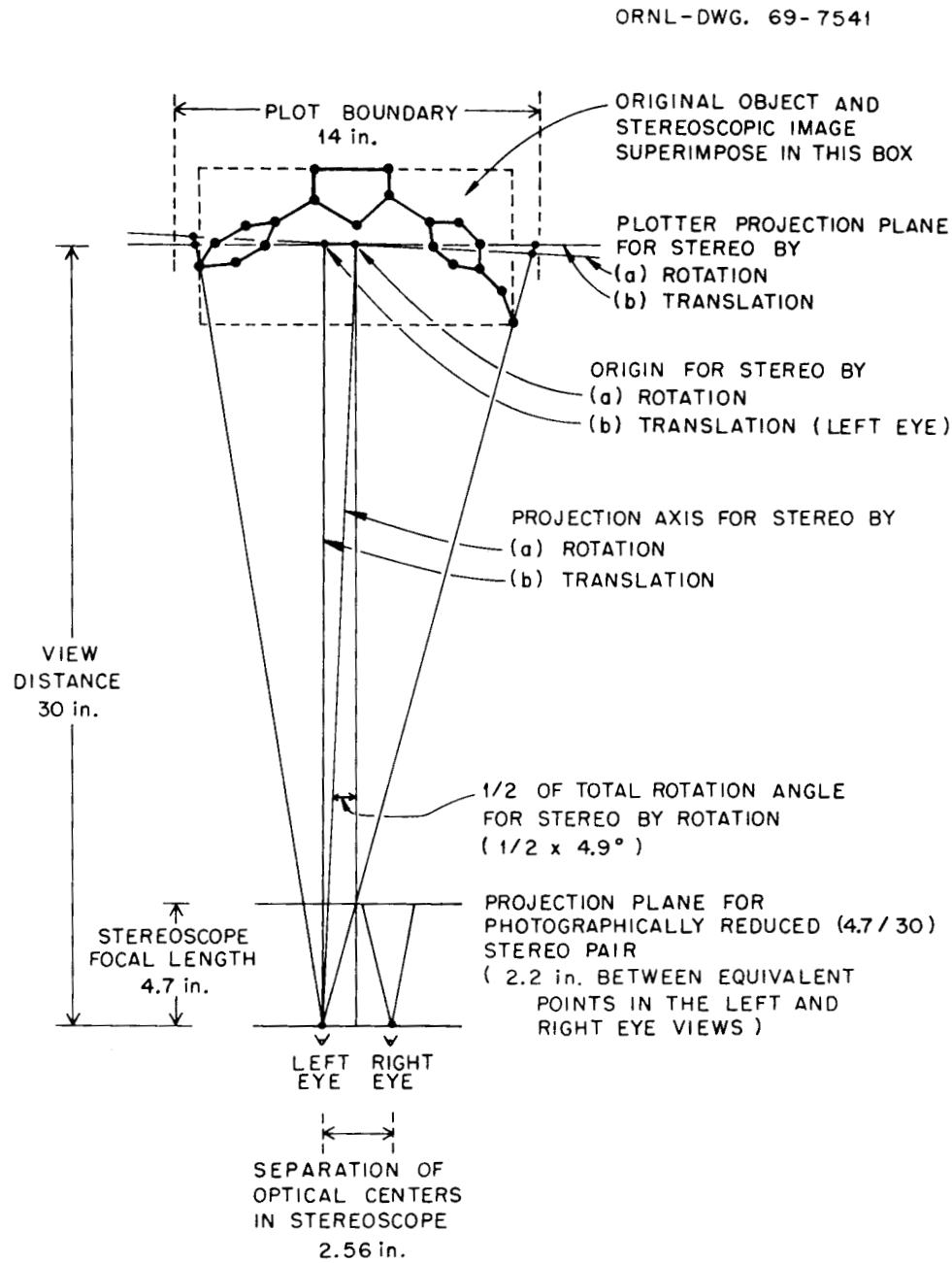

Fig. 3.1. Geometrical Relations Among the Stereoscopic Perspective Projection Parameters for a Typical OR TEP Drawing. The available plotting area for each projection is assumed to be 14 in. horizontally and at least 11 in. vertically. The scaled mathematical object is within a box 12 in. wide, 9 in. (or more) high, and 6 in. deep with the plane of the plotter halfway back into the box. The stereoscopic image seen through a stereoscope with a 12-cm (4.7-in.) focal length and a 6.5-cm (2.56-in.) separation between optical centers should appear superimposed on the original object. The parameters for both "translation stereo" and "rotation stereo" are shown. The appropriate linear dimensions can be scaled to accommodate other plotting areas and still produce the same final image.

ORNL DWG. 69-8122

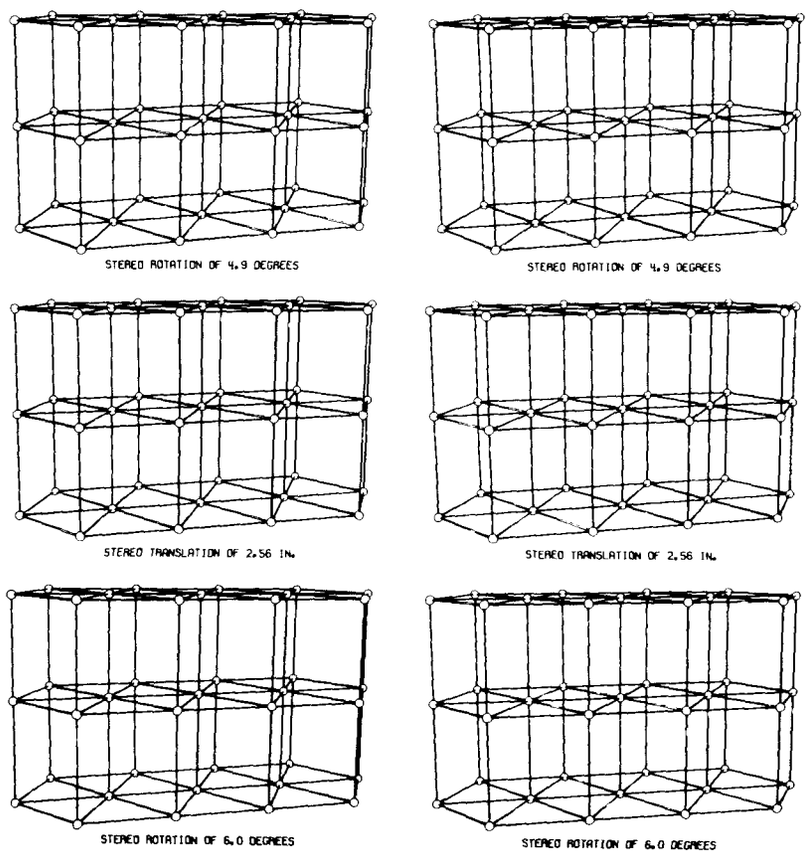

Fig. 3.2. Three Stereoscopic Drawings of a Hexagonal Lattice with Different Stereoscopic Parameters. The top and middle drawings utilize the parameters derived in Fig. 3.1 and demonstrate that the differences predicted (ref. 11) for translation and rotation stereo are not discernible in practice. The bottom stereo drawing illustrates the slight exaggeration in depth which occurs when a larger stereo rotation angle is used. The drawings should be viewed individually with a 12-cm focal-length stereoscope of good optical quality.

along the z-view direction is often minimized by this option. Furthermore, the x-y plane is the least-squares best plane for the atomic configuration. Format No. 2 trailer cards may be used to supply weights and screening (see Table 3.1).

3.3.6.7 Instruction 511, Overlap Elimination. – See Section 3.3.14.

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 instruction 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 instruction 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 equiprobability 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	–	–	8.5
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 viewpont. 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 3.3 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. 3.3, 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

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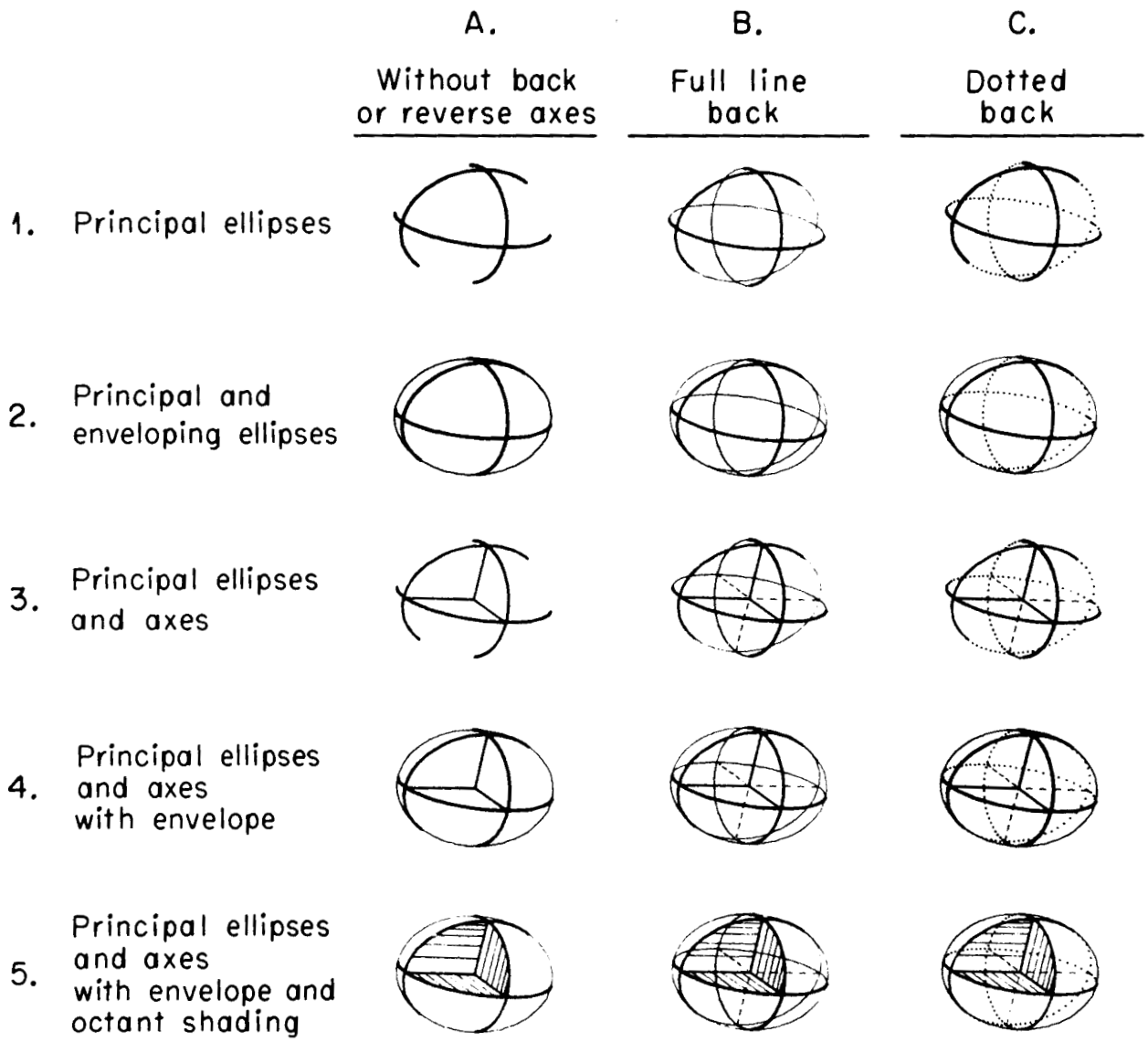

Fig. 3.3. Various Combinations of Ellipsoid Components.

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.

In order to distinguish certain atoms, such as those in disordered positions, a 705/715 instruction with NPLANE = 4, NDOT = 3, 4, 5, or 6, NLINE = 0, and NDASH = 0 may be used to produce dotted boundary ellipses to contrast with the normal solid line boundary ellipses. Another feature of the 705/715 instruction is that if NPLANE = 0, and if the symbol height is greater than zero, then chemical symbols alone are drawn on the atomic sites.

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) 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 $\Delta R(-5 \text{ in.}) = 0$, $\Delta R(5) = 0.008 \times (5 - 1) = 0.032$ in.; thus $A_0 = 0.016$ in. and $A_1 = 0.0032$ 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.

Selected types of atoms from the ATOMS table can be drawn without having to alter the contents of the table. This is accomplished by using an atom-number-run (ANR) code which includes the atom types that are to be drawn with a particular 700-series instruction. This feature is particularly useful when two or more different representations are used such as for the carbon and hydrogen atoms in the cubane example. If no ANR is entered, then all atoms in the table are drawn.

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 or atom selection is desired; otherwise 0)
4–9	701, 702, 703, 704, 711, 712, 713, 714
10–45	Blank
46–54	Symbol height (in.)
55–63	Parallel offset (in.)
64–72	Perpendicular offset (in.)
	Second Card (needed only for boundary retracing or atom selection)
1–3	Blank
4–9	Blank
10–18	A_0 (in.) or blank
19–27	A_1 (in.) or blank
28–36, 37–45	ANR or blank

3.3.8.2 Atom Plotting Instructions 705 and 715. –

Columns	
	First Card
1–3	1 (if boundary retracing or atom selection 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	Parallel offset (in.) } for symbols
64–72	Perpendicular offset (in.) } for symbols
	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., +, ×, *, 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.[12] 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 $-5 \leqq \text{NBOND} \leqq 5$. 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.

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

2. The bond radius (mean value for stick bonds) is in Angstrom units. Values between 0.01 and 0.06 A 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. The bond radius should not be made "vanishingly small" (e.g., $r < 0.005$ A) if the overlap feature is used because numerical rounding may cause incorrect hidden-line elimination.

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.

The use of vector-search-code (VSC) cards for the bond plotting instructions 802 and 803 has been extended to include a provision for drawing coordination polyhedra while suppressing the unwanted bonds. In addition to describing the bond with ANR(A), ANR(B), and the D min to D max range, a condition can be imposed to require that both atoms must be within a specified "polyhedral distance range" of an atom in the ATOMS table which has an atom number satisfying a third atom number run, ANR(P). This option is brought into play by a negative number in columns 43 to 48 of the VSC card and is applicable to instructions 802, 803, 812, and 813.

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 bonds are described with two atom designator codes for each bond. The atom designator codes go on the 801 card and on Format No. 1 trailer cards (see Table 2.1 for format). 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. In addition, a Format No. 2 trailer card is required with the fields specified under column 801 in Table 3.1 properly filled in.

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 and look ahead (2).

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).

The centered symbols drawn on the atomic sites by the 803/813 instructions may be made larger or smaller by redefining the SCAL2 factor, which is controlled by the 600 series of instructions (3.3.7).

3.3.9.4 Instructions 821 and 822, Overlap Elimination. See Section 3.3.14.

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 a 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 $P1$ 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 $P2$ is found by (*a*) translating from $P1$ 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 $P3$ is found by projecting $P2$ 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 $|x$ *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	*x* edge reset (in.)
37–45	*y* edge reset (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.

3.3.13 Supplementary Instructions (1200 Series). – These instructions utilize Subroutine SPARE.

3.3.13.1 Punching Cards with OR FLS Format. – An instruction 1201, which is implemented in subroutine SPARE, punches new position cards and temperature-factor cards with the format used by the OR FLS least-squares program. The instruction is useful for transforming a structure to a different asymmetric unit and for saving key atoms from a complex ATOMS array. First an ATOMS array is generated by the 400 series of instructions; then positional parameter cards, taken from the input atoms list, are read to define which atoms are wanted and to supply information about the scattering factor identifier and the multiplier. The parameter cards for all atoms in the ATOMS list which are crystallographically equivalent to the ones read are punched out. The sequence of the parameter cards read by this instruction need not correspond with the sequence of the original input atoms.

Columns

1–3 Blank

4–9 1201

10–18 *n* (the number of positional parameter cards to be read; *n* position parameter cards from the original input atom deck must follow this instruction card.)

3.3.14 Overlap Correction Instructions (511, 821, 822). – The hidden line correction feature of OR TEP-II eliminates most of the manual touch-up tasks previously required to correct for overlapping atoms and bonds. Drawings made with the overlap feature activated may require up to two or three times the computing time needed for noncorrected drawings; consequently, it is often more economical in computer time to make the preliminary drawings without overlap correction, particularly if a large number of atoms are present in the drawing.

To utilize the overlap feature an additional instruction, 511, is required, which is usually accompanied by type 2 trailer cards identical to those used by the 802 or 812 instructions. The 511 instruction stores the projected atom boundary ellipses for all atoms in the ATOMS list. It is important that the contents of the ATOMS list, the scaling and positioning, and the viewing parameters (controlled by the 400, 600, and 500 series of instructions respectively) not be changed between the 511 instruction and the drawing of the atoms and bonds by the 700 and 800 series of instruction; otherwise, the projected outlines may be destroyed or may be inappropriate.

The projected bond outlines, approximated as quadrangles, also may be stored for the overlap correction either by adding format No. 2 trailer cards to the 511 instruction or by using one or more 822 instructions (including those format No. 2 trailer cards) after the 511 instruction. The bonds to be stored are specified implicitly by the format No. 2 trailer cards. Explicit bonds also may be stored by using an 821 instruction (after the 511 instruction) with parameters identical to the 801/811 instructions to be used for plotting the explicit bonds.

The projected outline information for atoms and bonds must be recalculated for each member of a stereo pair; consequently the 511 and 821 or 822 instructions are usually the first instructions within the saved sequence. The old overlap information is removed whenever a new 500 or 600 series instruction is executed.

The maximum number of projected atoms and projected bonds which can be stored is 500 and 599 respectively. A list of the projected atoms and bonds is given in the printout.

An important feature of the OR TEP-II scheme for correcting overlap is that all details *inside* atoms and bonds, including chemical symbols and bond-distance labels, will be corrected for overlap; however, note that chemical symbols (drawn by the 700 series instructions and bond-distance labels (drawn by the 800 series instructions) which are *outside* the atoms or bond boundary *may not be corrected* for overlap. The reason for this is that the "area overlap search step" does not save projected atoms or bonds which do not contact the projected atom or bond to be drawn. Labels or symbols drawn with the 900 series instructions will not be corrected for overlap.

3.3.14.1 Instruction 511, Projected Outline Storage. – A constant width overlap margin (i.e., a blank strip at the intersection of overlapping elements) is included in the dimensions of each projected atom ellipse and projected bond quadrangle. The width of this margin may be specified as a parameter with the 511 instruction if desired; otherwise, the margin is set by default to either 0.025 inch or $(\mathrm{SCAL1})^{1/2} \times 0.030$ inch, whichever is largest. Some users prefer an overlap margin of 0.0 for stereoscopic drawings.

Columns	
1–3	2 (if bonds are to be stored; otherwise 0)
4–9	511
10–18	Blank or 0 – overlap margin default option described above 1 (or –1) – overlap margin = 0.0 $0 < \mathrm{OVMRGN} < 1.0$ – overlap margin = OVMRGN (in inches)

If column 3 is 2, format no. 2 trailer cards are included. In general all the trailer cards included with the 802/812 instructions are used.

3.3.14.2 Instruction 821, Explicit Bond Outline Storage. – If explicit bonds are to be stored for the overlap calculation, the attached atoms must be in the ATOMS list even though this is not a requirement for the 801/811 instructions used for plotting the explicit bonds. See 3.3.9.1 (Instructions 801 and 811) and Table 3.1 for description of parameters.

3.3.14.3 Instruction 822, Implicit Bond Outline Storage. – Normally the information on implicit bond outlines is stored with the 511 card; however, if more than 10 Format No. 2 trailer cards are needed, the extra ones can be entered with this instruction. All parameters are entered with the Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the 2 in column 3 and 822 in columns 7–9.

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 100 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 listed 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, SEARCH	Insufficient number of atoms in ATOMS list	EXIT
13	BOND	Imaginary bond intersection (i.e., bond larger than atom)	Omit bond
14	BOND	Hidden (end-on) bond	Omit bond
15	F900	Null vector as base line	Omit label
16	STORE	ATOMS list is full	Omit all succeeding atoms

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

Certain of the numerical procedures[1] 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 **V1**, **V2**, **V3** of the general ellipsoid and a vector **V4** from the center of the ellipsoid to the viewpoint. The vector **V5** normal to the polar plane (see Fig. 4.1), whose pole is the viewpoint, can be obtained from

$$\mathbf{V5} = \mathbf{A}\,\mathbf{V4}\ , \tag{4.1.1.1}$$

where **A** is the matrix for the ellipsoid which is defined by

$$\mathbf{X}^T\,\mathbf{A}\,\mathbf{X} = d\ , \tag{4.1.1.2}$$

where d is a constant.

The boundary ellipse is defined by two conjugate vectors, one of which is any vector **V6** perpendicular to **V5** and the second is **V7**, where

$$\mathbf{V7} = \mathbf{V5} \times \mathbf{A}\,\mathbf{V6}\ . \tag{4.1.1.3}$$

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).

[1]For a treatment of the projective and analytical geometry involved, the following four 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.

C. E. Springer, *Geometry and Analysis of Projective Spaces*, Freeman and Co., San Francisco, 1964.

J. A. Todd, *Projective and Analytical Geometry*, Pitman Pub. Corp., New York, 1946.

G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers*, McGraw-Hill Book Company, New York, 1961.

ORNL-DWG. 65-2671

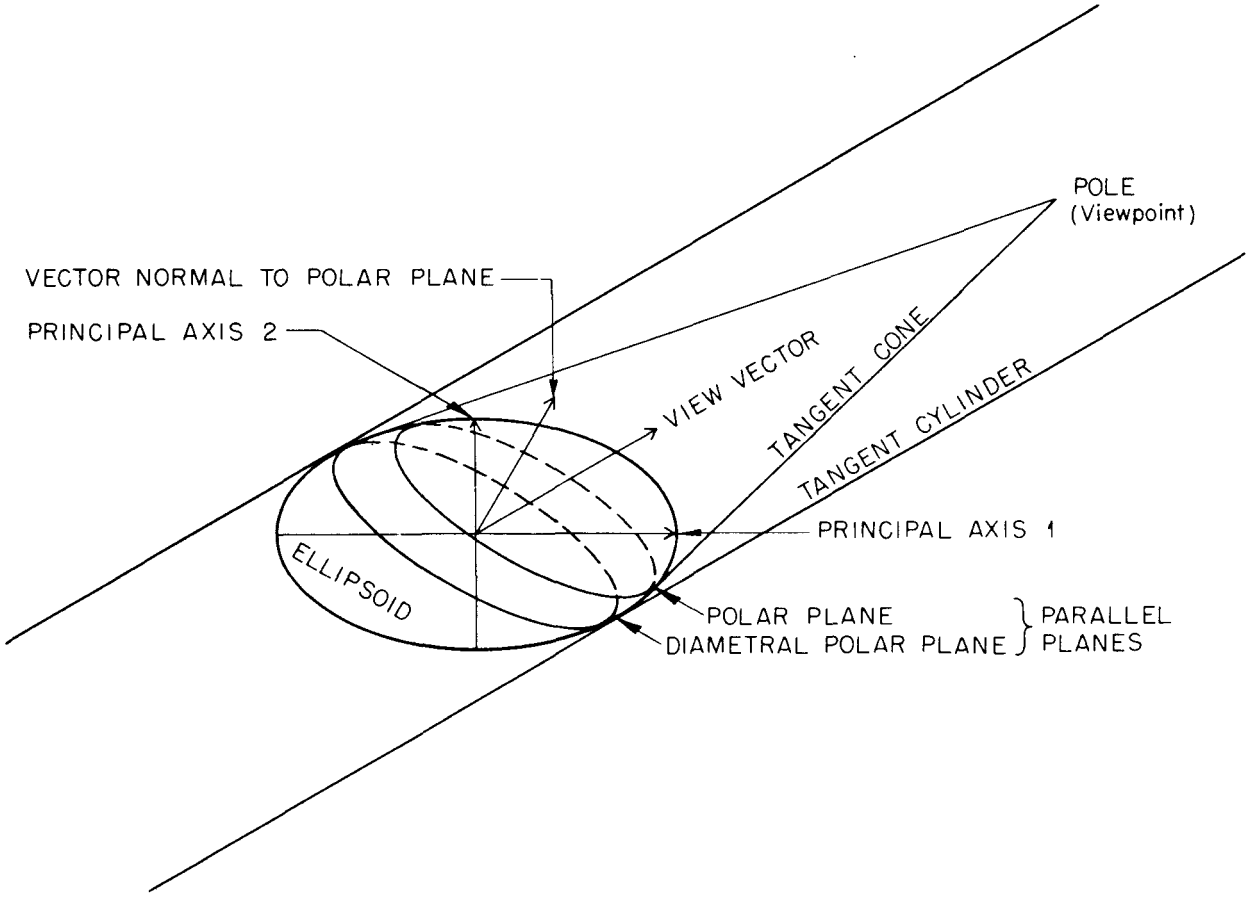

Fig. 4.1. Polar Planes Formed by Tangent Cylinder and Tangent Cone.

A principal ellipse which lies in the plane of the principal axis vectors **V1** and **V2** will have the third principal axis vector **V3** normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector **V8** where

$$\mathbf{V8} = \mathbf{V5} \times \mathbf{V3} \ . \tag{4.1.1.4}$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to **V8** and in the principal plane containing **V1** and **V2** is **V9**, where

$$\mathbf{V9} = \mathbf{V3} \times \mathbf{A}\,\mathbf{V8} \ . \tag{4.1.1.5}$$

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

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

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

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

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

$$\mathbf{X}^T \mathbf{A}\, \mathbf{X} = d\,, \tag{4.1.2.1}$$

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

$$\mathbf{X}^T \mathbf{B}\, \mathbf{X} = d\,, \tag{4.1.2.2}$$

where

$$\mathbf{B} = \begin{pmatrix} a_{11} - \dfrac{a_{13}a_{31}}{a_{33}} & a_{12} - \dfrac{a_{23}a_{31}}{a_{33}} & 0 \\ a_{12} - \dfrac{a_{13}a_{32}}{a_{33}} & a_{22} - \dfrac{a_{23}a_{32}}{a_{33}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.1.2.3}$$

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 **l** parallel to **Vb** and let

$$\mathbf{X}_j = \mathbf{Vr}_j + s\,\mathbf{l}\,, \tag{4.1.2.4}$$

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

$$s^2 \mathbf{l}^T \mathbf{A}\,\mathbf{l} + 2s\,\mathbf{Vr}^T \mathbf{A}\,\mathbf{l} + \mathbf{Vr}^T \mathbf{A}\,\mathbf{Vr} - d = 0\,; \tag{4.1.2.5}$$

solving for s we get

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

The elliptic cone which is tangent to the ellipsoid and which has its apex on the viewpoint can be obtained from the matrix **A** and from the vector **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 **Vu**.
2. The tangent cone can now be described as

$$\mathbf{Y}^T \mathbf{C}\,\mathbf{Y} = 0\,, \tag{4.1.2.7}$$

where **Y** is a vector originating from the vertex (viewpoint) of the cone and

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

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

$$\mathbf{Y} = \mathbf{Vp} + s\,\mathbf{l} \tag{4.1.2.9}$$

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

$$s = \frac{-\mathbf{V_p}^T \mathbf{C}\,\mathbf{l} + \sqrt{(\mathbf{V_p}^T \mathbf{C}\,\mathbf{l})^2 - (\mathbf{l}^T \mathbf{C}\,\mathbf{l})(\mathbf{V_p}^T \mathbf{C}\,\mathbf{V_p})}}{\mathbf{l}^T \mathbf{C}\,\mathbf{l}} \tag{4.1.2.10}$$

The vector $\mathbf{V_p}$ from the vertex to $\mathbf{p}$ 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 $NJ \geqq 12$. $NJ = \text{instruction}/100$.

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 $\neq 0$; 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 ($1 \leqq$ ND $\leqq 5$).

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

4.2.2.12 LAP500. – This routine sorts the ATOMS list, then calculates the projected outline ellipses for all atoms in the ATOMS list. The ellipses are stored in the CONIC array along with the minima and maxima in x and y for a rectangle enclosing each ellipse.

4.2.2.13 LAP700. – This routine finds the atoms which overlap a given atom to be drawn. The routine first checks the bounding rectangles for intersections, then forms the cubic discriminant from the quadratic descriptions of the two projection ellipses. The discriminant provides a specification for complete overlap, partial overlap or no overlap. A list of up to 20 interfering ellipses is compiled.

4.2.2.14 LAP800. – This routine is used in the "Projected Outline Storage Step" to store the projected quadrangles for the bonds specified by the trailer cards of the 511, 821, and 822 instructions. The routine also is used in the "Area–Overlap Search Step" to find the projected bond quadrangles which overlap a given bond to be drawn. A list containing up to thirty interfering quadrangles is compiled.

4.2.2.15 LAPAB. – This routine finds the bonds that overlap an atom to be drawn and the atoms that overlap a bond to be drawn. It is used in the "Area–Overlap Search Step."

4.2.2.15 LAPDRW. – This routine checks each line segment to be drawn for intersection with the interfering ellipses and quadrangles and compiles a list of intersections. The intersection list is sorted according to distance along the line segment, and the intersection pattern is analyzed to determine which subsegments are visible and which are hidden. The line subsegments are passed to the SCRIBE routine.

4.2.2.17 SCRIBE. – This routine filters out the hidden line segments and passes the visible line segments to the DRAW routine.

4.2.3 Arithmetic Subprograms. – 4.2.3.1 Function ARCCOS (X). – This routine computes θ, the arc cosine of X in degrees; $0 \leqq \theta \leqq 180°$.

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 $\leqq 0$: triclinic system

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

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

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 **A B** = **C**. The location of **C** must be different from **A** and **B**.

4.2.3.7 MV (A,X,Y), DIMENSION A(3,3),X(3),Y(3). – MV performs the matrix-vector multiplication **A X** = **Y**. The location of **Y** must be different from **A** and **X**.

4.2.3.8 NORM (X,Y,Z,ITYPE), DIMENSION X(3),Y(3),Z(3). – NORM stores at **Z** a vector (not necessarily a unit vector) perpendicular to both **X** and **Y**. The sense of **Z** is that of the vector product **X** × **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 **C** must be different from **A** and **B**.

4.2.3.10 UNIT (X,Y,ITYPE), DIMENSION X(3),Y(3). – The vector **Y** is made 1 A long and parallel to **X**. The vectors **X** and **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 **Y** must be different from **X** and **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 $\mathbf{X}^T\mathbf{A}\ \mathbf{Y}$ = scalar.

4.2.3.13 FUNCTION VV (X,Y), DIMENSION X(3),Y(3). – VV performs the vector-vector multiplication $\mathbf{X}^T\mathbf{Y}$ = 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 NUMBUR.

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(1500)

and card F2000180 contains

"210 CALL PLOTS (PLA,1500, LTNO)"

for the CDC 1604-A or

"210 CALL PLOTS (PLA(1500),1500,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 DRAW0330 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 $N \geqq 0$)

   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 $^4/_7$ the height and the character spacing is $^6/_7$ 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 $0 \leqq NUM \leqq 14$ 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.

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

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

ENTRY – NUMBUR(X(1),X(2),H,A,THETA,N)

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.

N is the number of digits to the right of the decimal point. A(–1) value will suppress the decimal point.

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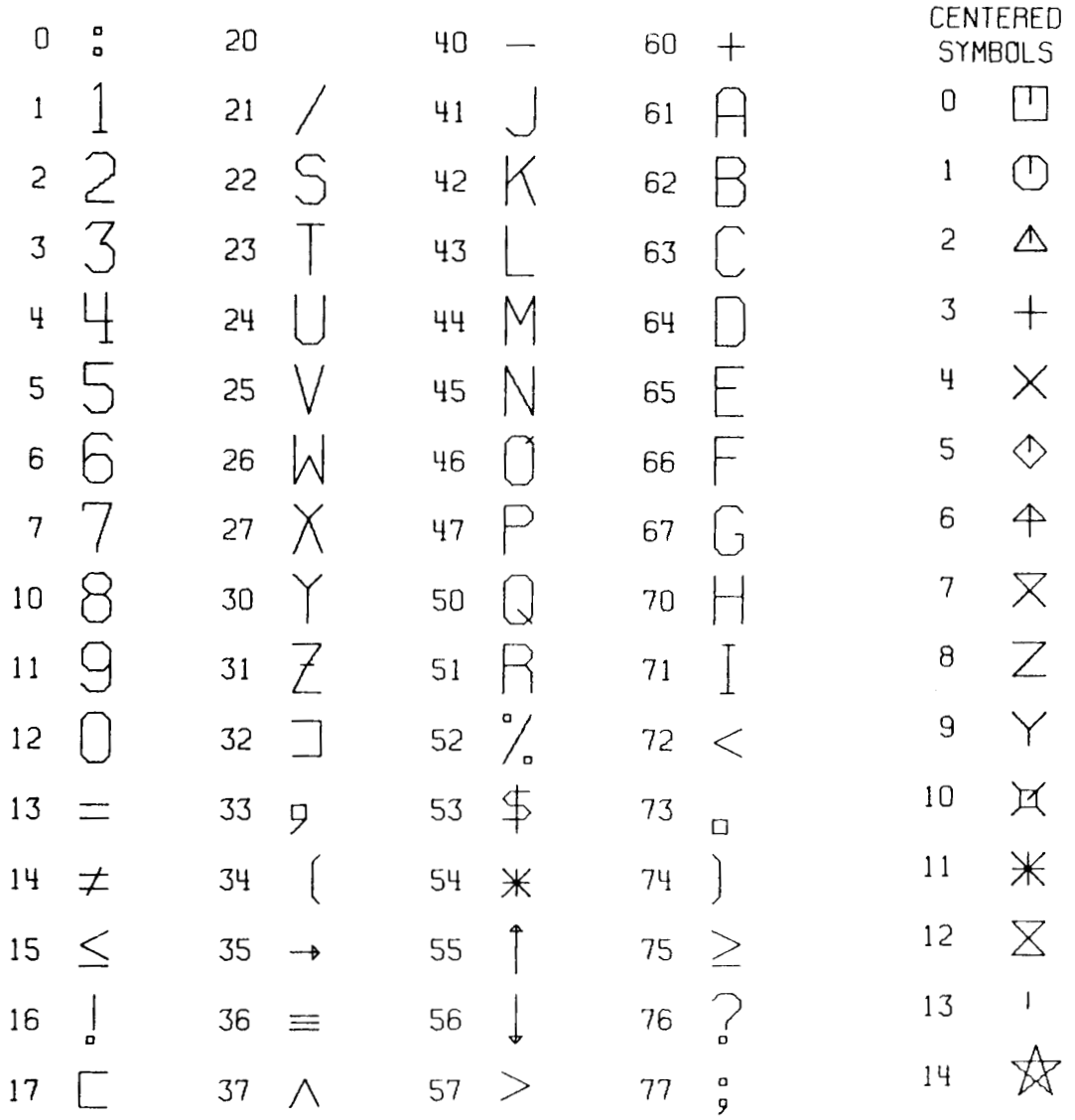

Fig. 4.2. Characters Available in 1604-A Symbol Routine.

4.3 Adapting OR TEP to Other Equipment Configurations

Card images[2] for OR TEP will be provided to crystallographers and others who request that the program be sent to them.

FORTRAN decks are available in IBM 360 FORTRAN IV and IBM 7090 FORTRAN IV. The FORTRAN subprograms are arranged alphabetically within the FORTRAN source decks. An exception is MAIN, which is first in each deck.

[2]The size of the card deck (3000–6000 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 an agreed upon format and the tape returned to the sender.

The machine language subroutines SIMBOL and NUMBUR are modifications of the CalComp subroutines SYMBOL and NUMBER. Subroutine PLOT is an unmodified CalComp subroutine also written in machine language. These three subroutines are copyrighted by California Computer Products, Inc. Subroutines SIMBOL and NUMBUR for IBM 360, IBM 7090, and CDC 1604-A can be distributed from ORNL. Subroutine PLOT which is different for each plotter may be obtained from California Computer Products, Inc., 305 Muller Avenue, Anaheim, California (Attention: Programming Dept.).

Cards for the example figure, cubane, will be included with the deck.

4.3.1 OR TEP Source Deck Differences for the IBM 360 and the IBM 7090. – The listing of the FORTRAN IV source deck for the IBM 360 is given in Sect. 7. The length of the single-precision floating-point word in the IBM 360 is such that the maximum number of atoms in the input list cannot be greater than 166 because of the way the atom designators are stored. This must be taken into account if the dimension statements of the program are changed.

The following changes are made to modify the program for IBM 7090 FORTRAN IV:

1. Remove the "REAL*8 CHEM" card from the subprograms which use common.
2. Add the correct IBSYS monitor control cards including "$POOL" and "$GROUP" cards to conserve memory space.

The following changes are made to modify the program for IBM 7090 FORTRAN II:

1. Remove the "REAL*8 CHEM" cards from the subprograms which use common.
2. Add "*LIST8" and "*LABEL" cards before each subprogram.
3. Replace card F2000180 with "210 CALL PLOTS (PLA(1500), 1500,LTNO)."
4. Change input-output statements and library function names to correspond with FORTRAN II convention.

4.3.2 External Device Logical Number Assignments. – Logical device 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	=	5	PRIM0220
b) Monitor Output	NOUT	=	6	PRIM0280
c) Scratch	NSR	=	8	PRIM0290
d) Plotting	LTNO	=	23	(PRIM0250)*

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

*In the present revision, LTNO also serves as a plotting device indicator and is initialized to zero at MAIN0145. For the mechanical plotter (CRT), LTNO is set to 15 (–99) at F2000210 (F200250) by a 201 (203) instruction.

the 200 series instructions may have to be redefined and expanded to accommodate the rules of the new system.

Location DRAW0330 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 IBM 360, IBM 7090, and CDC 1604-A. – Basically, the OR TEP system is designed to be used in a 32 K memory. Consequently, OR TEP would have to be changed considerably to operate in a much smaller memory.

The FORTRAN coding of OR TEP has proven to be fairly machine independent, but as compilers become more sophisticated new problems continually appear. For example, some compilers rearrange the sequence of operations to obtain more efficient execution and sometimes they "outsmart" themselves in the process. Certain of the 6000 series CDC compilers occasionally take an instruction such as I1 = ATOMS(1, J) / 100000. and make it into TEMP = 1./100000.; I1 = ATOMS(1,J)*TEMP. The effect is disastrous because the numerical rounding and truncation produce an incorrect integer I1.

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

SIMBOL is called from BOND0460, BOND0480, F7000850, F9001310, F9001340, and F9001470.

NUMBUR is called from BOND 2510 and F9001440.

4.3.5 Space Requirements with Overlap Feature. – The overlap feature requires an additional block of approximately 15 K words of computer memory and will cause ORTEP to exceed the memory of a 32 K computer. For computers with a working storage under 45 K–60 K words, the overlap feature may be deleted by removing subroutines LAP500, LAP700, LAP800, LAPDRW, LAPAB, and LAPCON and substituting dummy subroutines for the first four of these six subroutines.

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 $\geq$ 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 α, cos β, cos γ, $\alpha(°)$, $\beta(°)$, $\gamma(°)$.
	AA(3,3)	Metric tensor **g** where $\mathbf{g}_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.
	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(8,10)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(100)	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(3,100)	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(5,10)	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.
P	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).
	P(3,100)	Triclinic positional coordinates for the input atoms.
	PA(3,3,100)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 A 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 A 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 A 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. $\mathbf{REFV}^T = \mathbf{AAREV}^{-1}$.
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.

$x \geqq$ Res(1)	128-point ellipse
Res(1) $> x \geqq$ Res(2)	64-point ellipse
Res(2) $> x \geqq$ Res(3)	32-point ellipse
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 used to transfer Z coordinates to subroutine DRAW when perspective lettering is 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 Lana[5] and the handbooks by Burington and May[6] and Owen[7] 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

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

If the integration is carried over all space, then

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

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

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

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.

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

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

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

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

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

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

[7] D. 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

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

where

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

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

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

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,

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

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

$$\Phi(\mathbf{T}) = \exp\left[i\mathbf{T}^T\hat{\mathbf{X}} - \tfrac{1}{2}\mathbf{T}^T\mathbf{M}\mathbf{T}\right] , \tag{5.3.2}$$

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

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

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

[a]Reproduced 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 nth 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

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

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

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

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

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

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

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

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

$$\mathbf{y}^T\mathbf{G}^{-1}\mathbf{M}^{-1}\mathbf{y} = 1 , \tag{5.4.2}$$

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

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

[10] D. 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 $\mathbf{a}_i \cdot \mathbf{a}_j$ and $\mathbf{a}_i \cdot \mathbf{a}_j$ is the scalar vector product of two of the three unit cell vectors. Introducing the Lagrange multiplier $1/\lambda$ leads to

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

premultiplying by $\mathbf{M}$ yields

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

Or we can do some additional rearranging and obtain

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

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 $\mathbf{M}\mathbf{G}^{-1}$ 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 O_3.

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 isocitrate[3] 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-inositol[4] 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.

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[1] C. K. Johnson, *Acta Cryst.*, 18, 1004 (1965) .

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

[3] D. van der Helm, J. P. Glusker, C. K. Johnson, J. A. Minkin, N. E. Burow, and A. L. Patterson, *Acta Cryst.*, B-24, 578 (1968).

[4] I. 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 hydrate[5] 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 sucrose[6] 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 structure[7] 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 Larson[8] 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 acid[11] (cis, D, L-8,9-methylene-heptadecanoic 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.

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[5] G. M. Brown and H. A. Levy, *Cryst. Struct. Commun.* **2**, 107 (1973).

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

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

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

[9] H. G. Smith, S. W. Peterson, and H. A. Levy, *J. Chem. Phys.* **48**, 5561 (1968).

[10] R. D. Ellison and H. A. Levy, *Acta Cryst.*, **19**, 260 (1965).

[11] G. 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) Acetylacetonate. – Dr. Bruno Morosin from Sandia Corporation sent this most unusual example of thermal motion. Cr(III) acetylacetonate[15] has three acetylacetonate 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 structure[10] 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

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

[13] G. E. Gurr, *Acta Cryst.* B24, 1511 (1968) and private communication, 1964.

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

[15] B. Morosin, *Acta Cryst.* 19, 131 (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 model[18] 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]

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

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

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

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

ORNL DWG. 65-2448

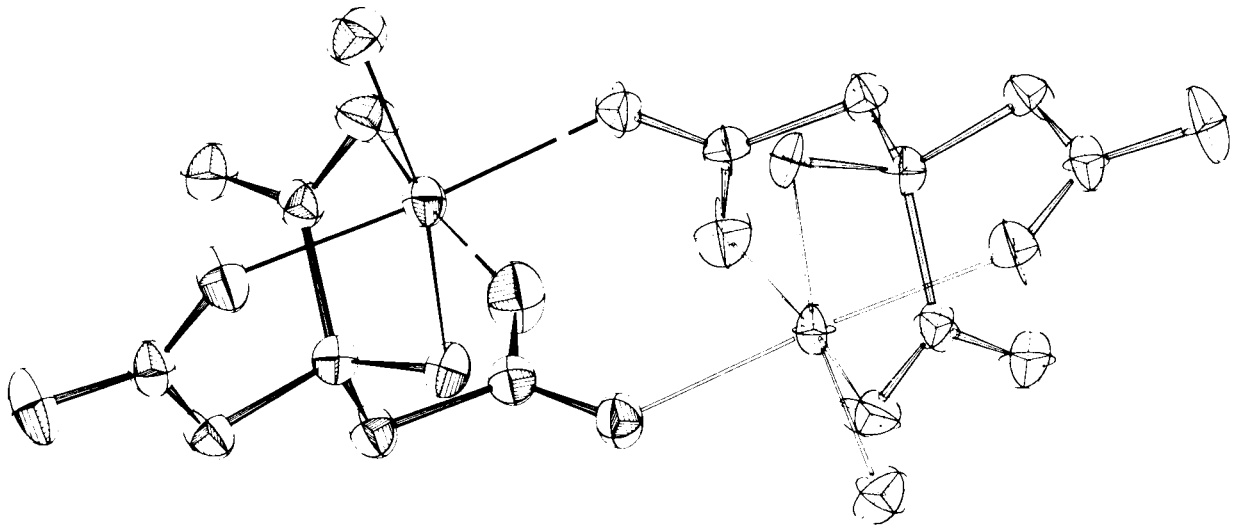

Fig. 6.1. Chelation Pattern Viewed Along a Twofold Screw Axis in the Crystal Structure of Magnesium Citrate Decahydrate. Ellipsoids represent equiprobability surfaces of thermal displacement and contain 65% of the probability distribution.

ORNL DWG. 65-2443

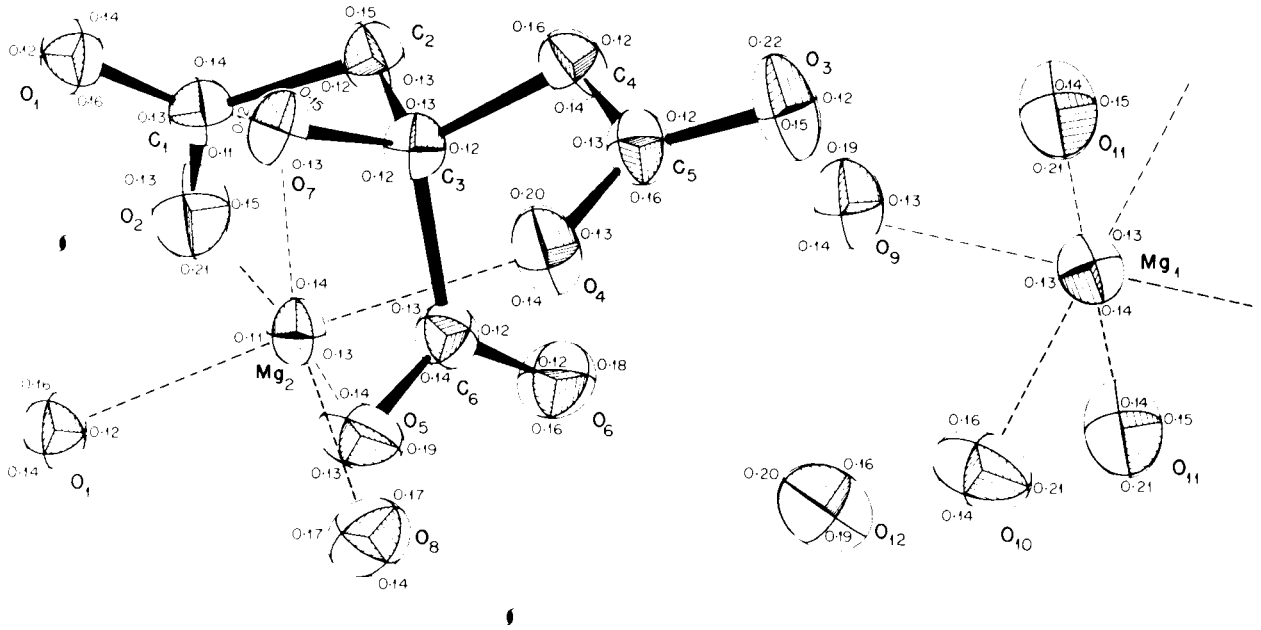

Fig. 6.2. Thermal-Ellipsoid Representation for Magnesium Citrate Decahydrate with Principal Values of RMS Displacement in Angstrom Units. Ellipsoids enclose 74% probability. Structure is viewed along *b* axis.

ORNL DWG. 65-2444

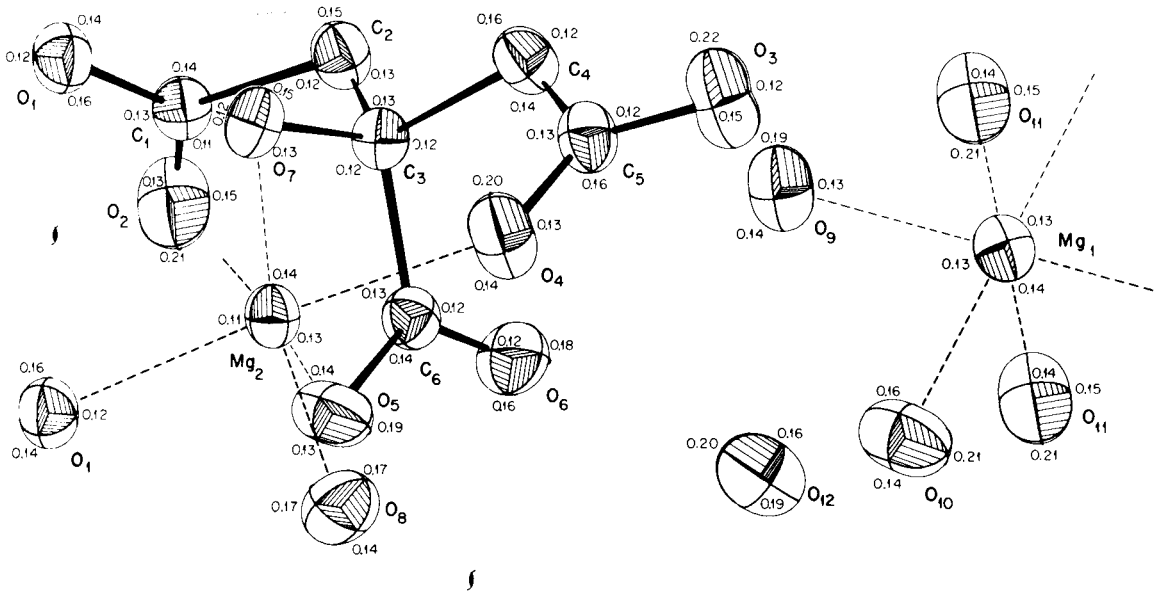

Fig. 6.3. Peanut-Shaped RMS Thermal-Displacement Figure Representation for Magnesium Citrate Decahydrate. Principal values of rms displacement in Angstrom units are indicated around the displacement figures, which are drawn at double scale. Same view of structure as shown in Fig. 6.2.

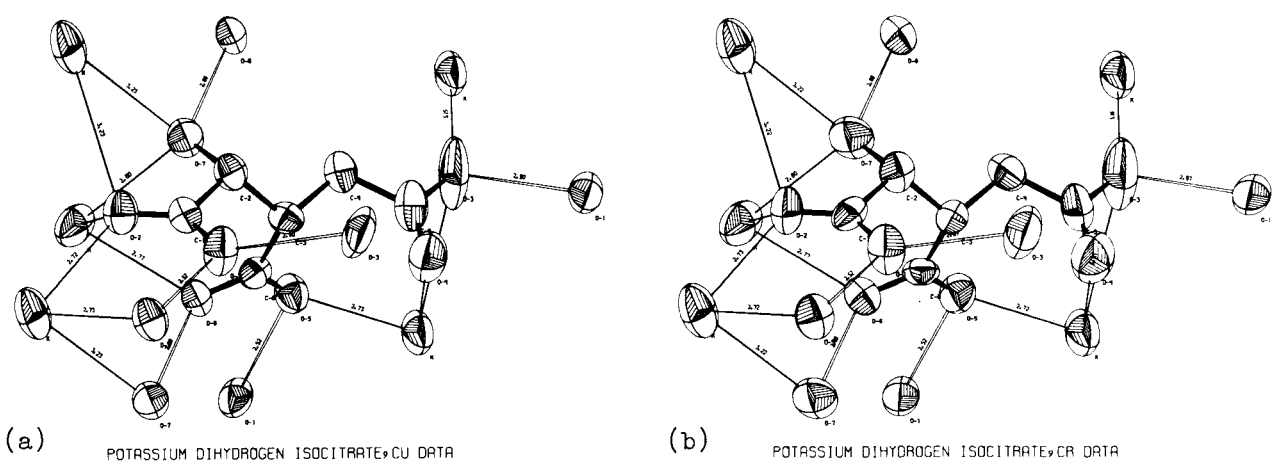

Fig. 6.4. Potassium Dihydrogen Isocitrate with Thermal Ellipsoids Scaled to Include 74% Probability. (*a*) Results obtained from 1350 three-dimensional copper K_α data (disagreement factor 6.5%). (*b*) Results obtained from 340 three-dimensional chromium K_α data (disagreement factor 2.2%). Note: This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

ORNL DWG. 65-2450

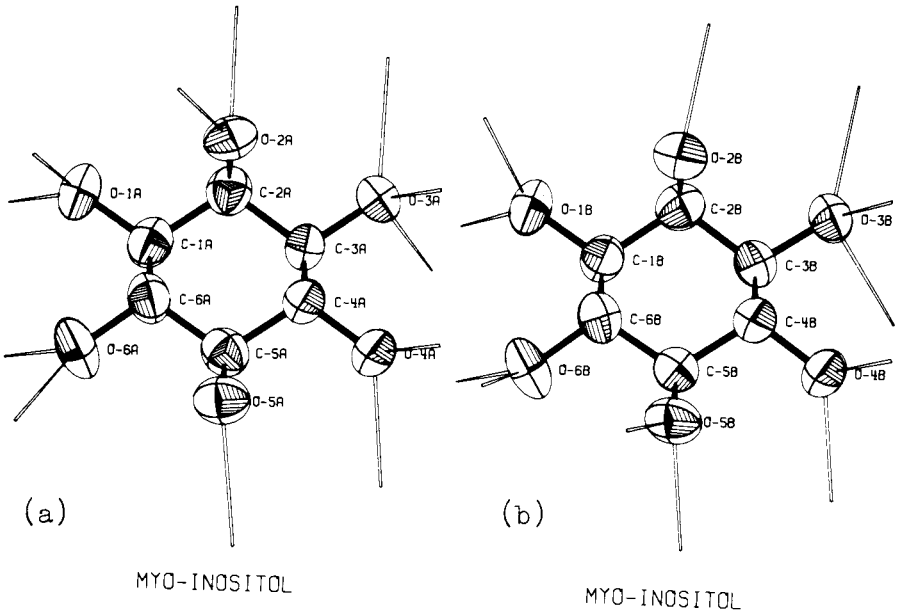

Fig. 6.5. Comparison of Thermal Ellipsoids in the Two Crystallographically Independent Molecules of Myo-Inositol (6.5*a* and 6.5*b*). Hydrogen bonding is shown, since this might influence the thermal motion. Ellipsoids are scaled to include 74% probability. Note: This is *not* a stereo pair.

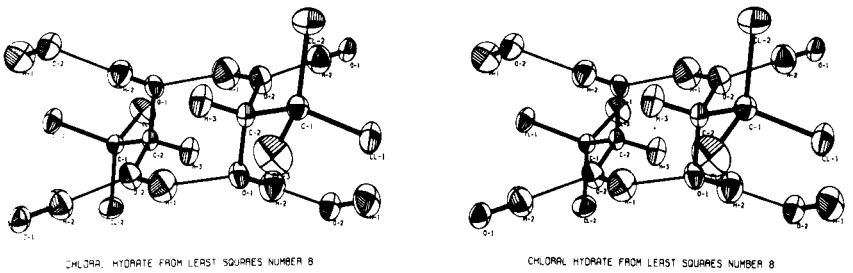

Fig. 6.6. Stereogram (Stereoscopic Pair of Perspective Projections) of Chloral Hydrate Viewed Along the Reciprocal Axis a^*. Two molecules are shown related by a center of symmetry, with the hydrogen bonds connecting them together and to other molecules. Ellipsoids are scaled to include 48% probability.

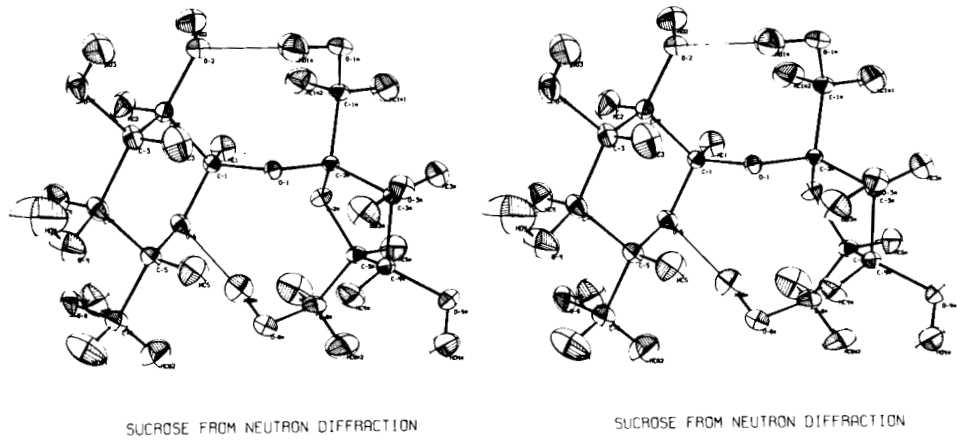

Fig. 6.7. Stereogram Showing the Sucrose Molecule with Thermal Ellipsoids Scaled to Enclose 50% Probability.

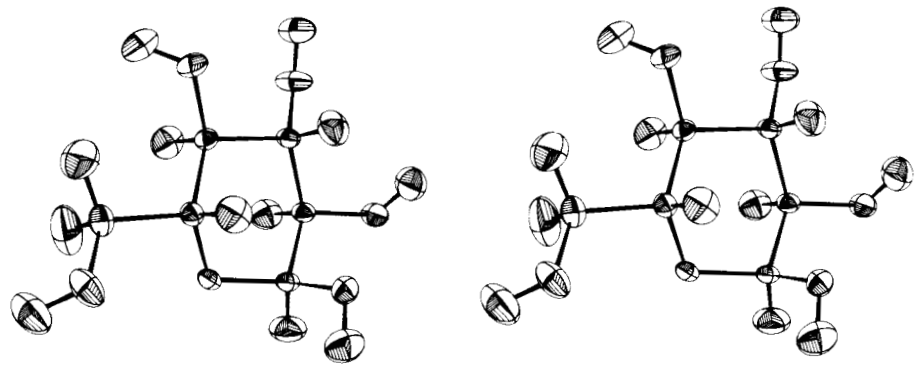

Fig. 6.8. A Molecule of Glucose with Thermal Ellipsoids Scaled to Enclose 50% Probability.

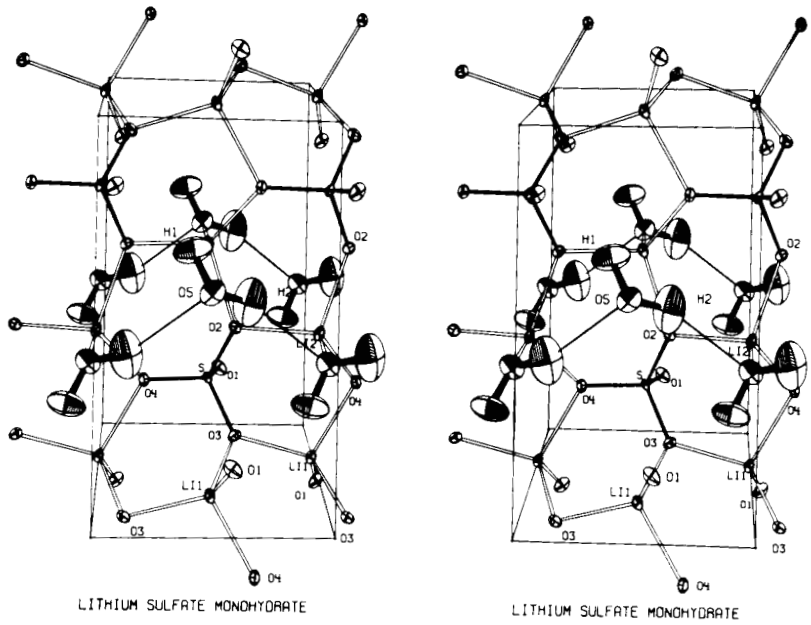

Fig. 6.9. Lithium Sulphate Monohydrate. The lithium ions and sulphate ions are coordinated into a compact network. The structure is viewed along the reciprocal a^* axis. The ellipsoids are scaled to enclose 20% probability.

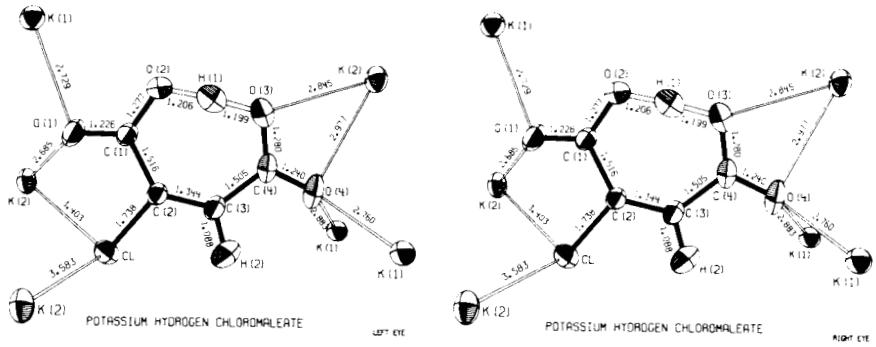

Fig. 6.10. Potassium Hydrogen Chloromaleate. The chloromaleate ion is viewed normal to its own plane. The thermal ellipsoids enclose 50% probability.

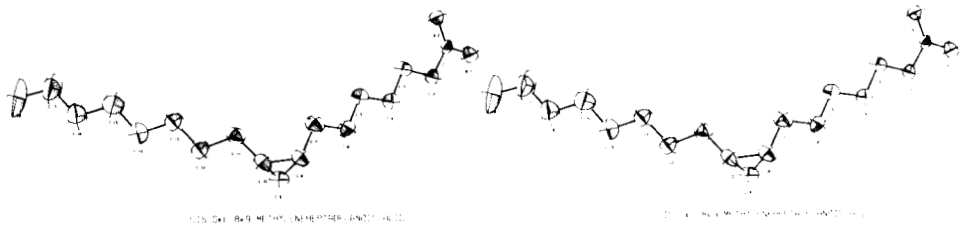

Fig. 6.11. A Molecule of Dihydromalvalic Acid with Thermal Ellipsoids Scaled to Enclose 48% Probability.

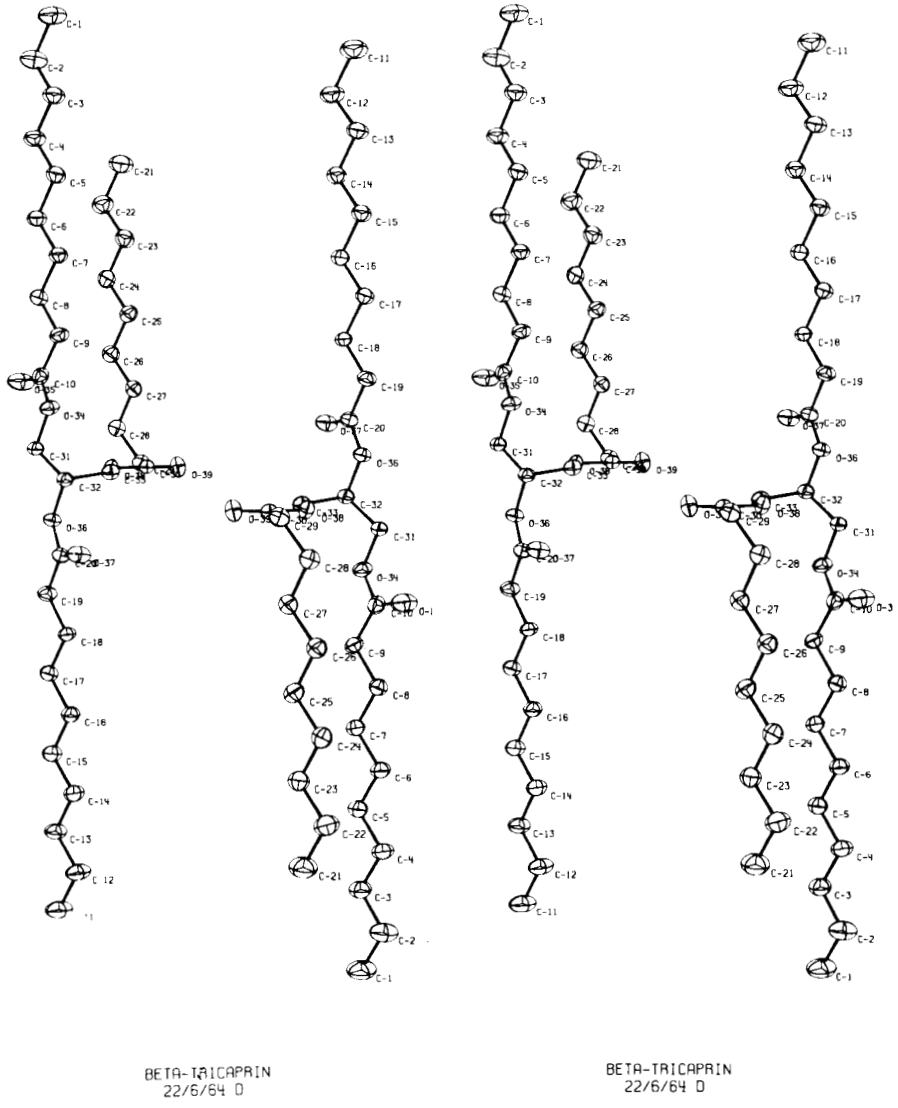

Fig. 6.12. Two Molecules of Beta-Tricaprin Related by a Center of Symmetry. The thermal ellipsoids are scaled to include 30% probability.

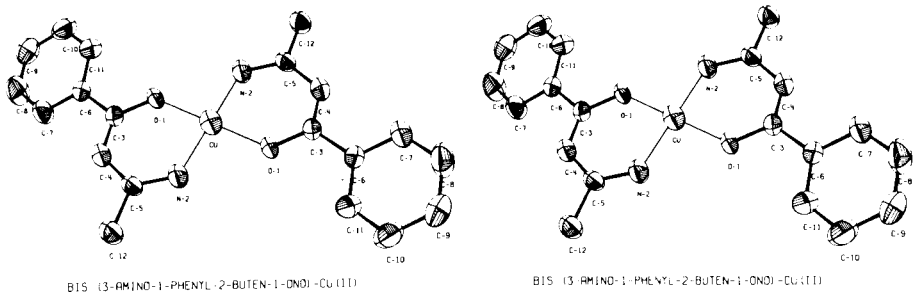

Fig. 6.13. Chelation Complex of *Bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

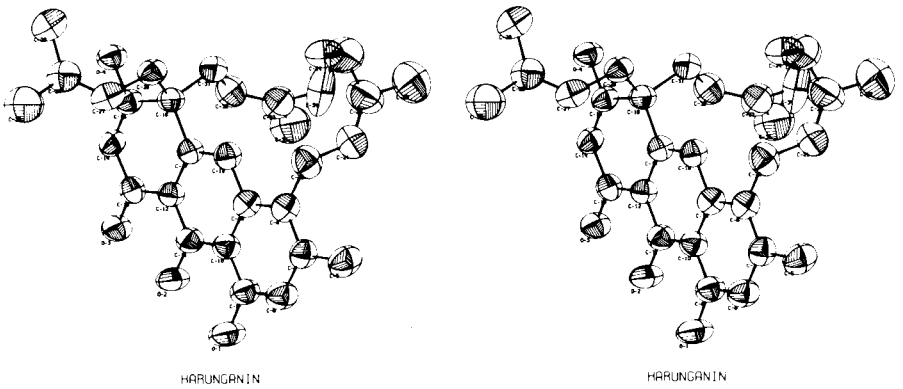

Fig. 6.14. A Molecule of the Plant Pigment Harunganin with Thermal Ellipsoids Scaled to Include 48% Probability.

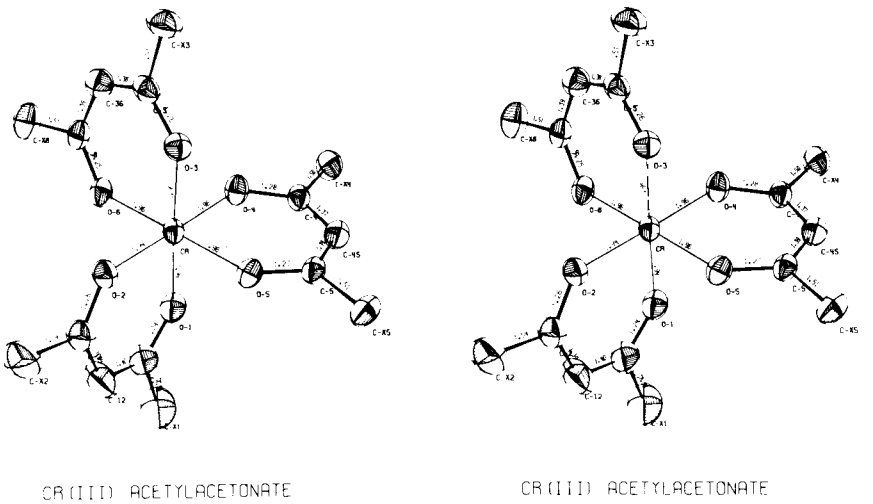

Fig. 6.15. A Unit of *Tris*-acetylacetonatochromium(III) Viewed Along its Threefold Axis of Chemical Symmetry. The thermal ellipsoids are scaled to enclose 20% probability.

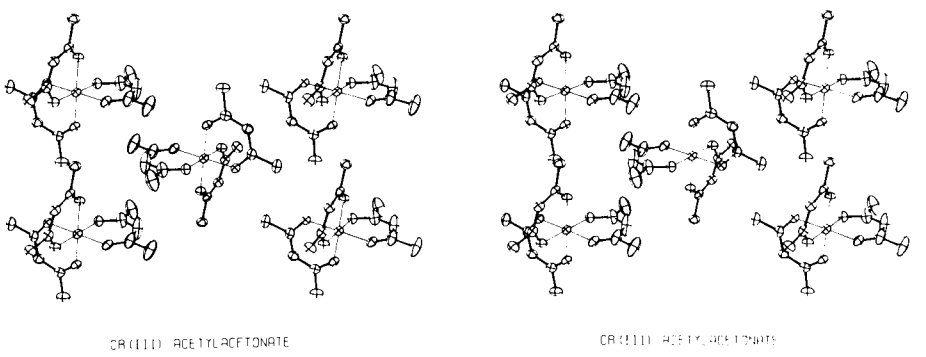

Fig. 6.16. Packing Diagrams for *Tris*-acetylacetonatochromium(III) Viewed Along the Reciprocal Axis c*. Thermal ellipsoids are scaled to enclose 20% probability.

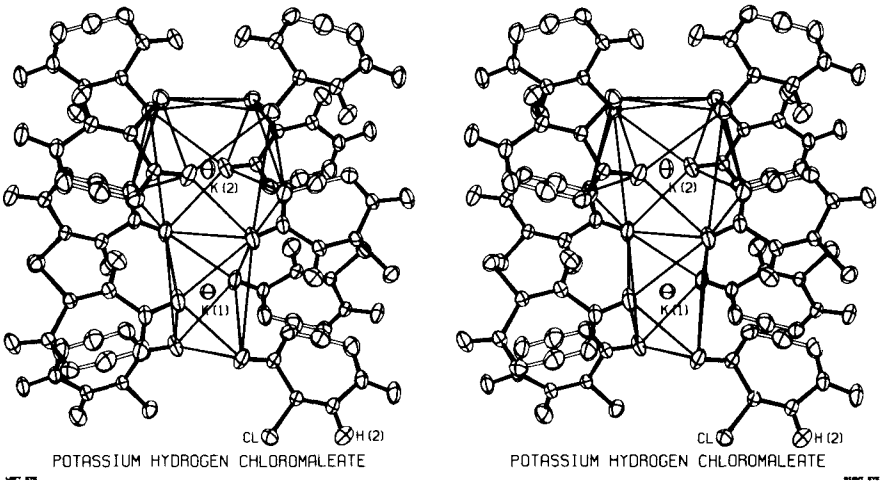

Fig. 6.17. Packing of Chloromaleate Ions Around the Potassium Ions in Potassium Hydrogen Chloromaleate. The edges of the coordination polyhedra are shown. View is nearly along the *c* axis. Thermal ellipsoids are scaled to contain 50% probability.

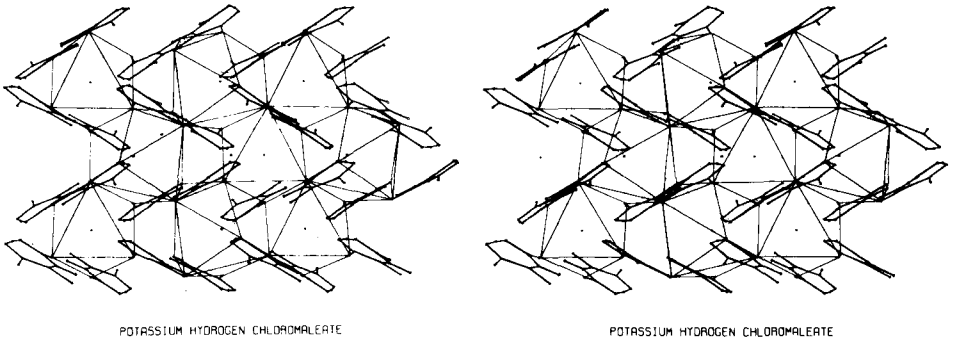

Fig. 6.18. Packing Diagrams for Potassium Hydrogen Chloromaleate. Atoms are represented as small circles. The edges of the coordination polyhedra around the potassium ions are shown. View is nearly along the *a* axis.

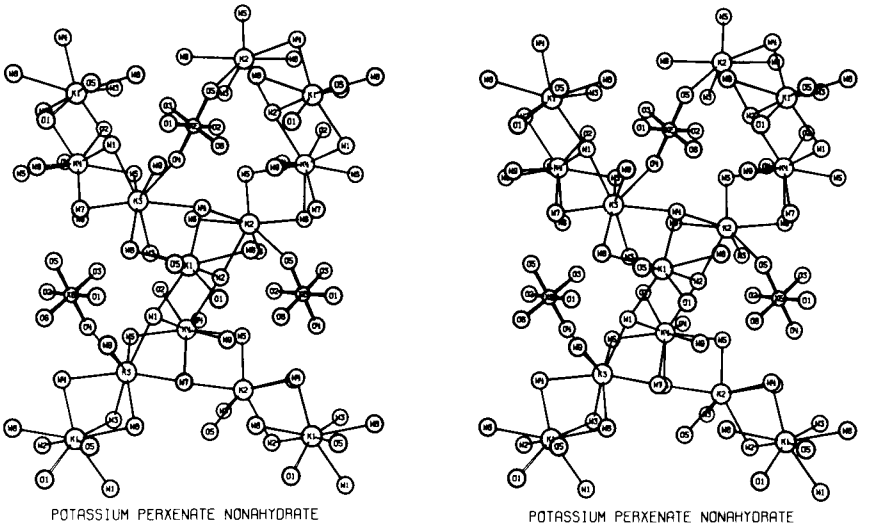

Fig. 6.19. Packing Diagram for Potassium Perxenate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Perxenate Ions. The view is parallel to the *a* axis. Another layer, related to the present one by a twofold screw axis along *a*, is needed to complete the structure.

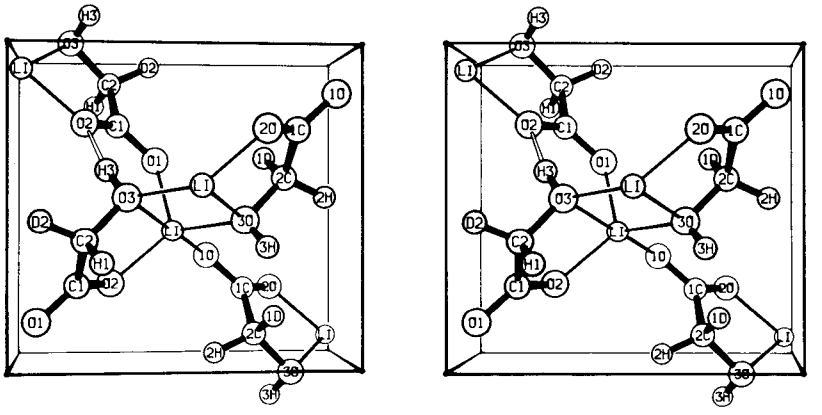

Fig. 6.20. A Stereogram Showing the Unit-Cell Contents of Anhydrous Li α-monodeuteroglycolate. The unique monoclinic *b* axis points up in the page and the mean *c* axis out from the page.

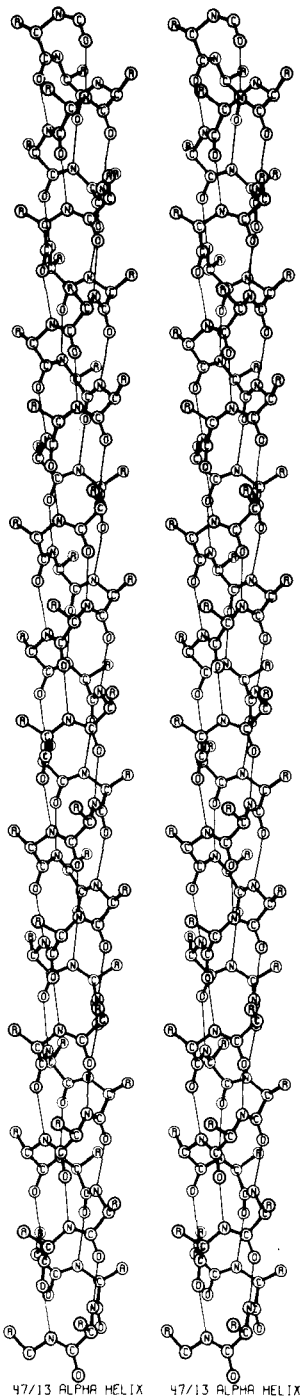

Fig. 6.21. A Stereoscopic Pair of Perspective Projections Showing the Alpha-Helix Which Is Present in Poly-L-Alanine. There are 47 amino-acid residues in 13 turns of the helix. Stereo viewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP-II

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C     TOTAL NUMBER OF CARDS INCLUDING DATA FOR EXAMPLE IS 4745          MAIN  10
C     ***** OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM ****               MAIN  20
C     ***** ORTEP-II / IBM-360 / FEB 1971 / INSTRUCTIONS IN CRNL-3794 **MAIN  30
C     ***** OPTIONAL OVERLAP FEATURE ADDED TO ORTEP IN FEBRUARY 1971 ***MAIN  40
C     ***** CUBANE EXAMPLE CARDS ILLUSTRATE USE OF OVERLAP FEATURE *****MAIN  50
C     ***** IN BRIEF, INSTRUCTION 511 MAY BE USED JUST BEFORE EACH      MAIN  60
C     ***** DRAWING TO STORE THE PROJECTED ATOMS, TYPE 2 TRAILER CARDS  MAIN  70
C     ***** WITH INSTR 511 CAUSES PROJECTED BONDS ALSO TO BE STORED     MAIN  80
C     ***** MAXIMUM NUMBER OF STORED BONDS IS 599.  IN GENERAL, JUST USEMAIN  90
C     ***** THE SAME TYPE 2 TRAILER CARDS USED BY THE 802/812 INSTR. ***MAIN 100
C     ***** COLS 10-18 ON 511 INST CARD SPECIFIES OVERLAP MARGIN(OVMRGN)MAIN 110
C     *****          0        OVMRGN = MAX(0.035 OR SQRT(SCAL1)*0.030)  MAIN 120
C     *****       1 OR -1     OVMRGN = 0.0                              MAIN 130
C     *****    .GT.0,.LT.1  OVMRGN = ACTUAL VALUE GIVEN (INCHES) *****  MAIN 140
C     ***** ALL OVERLAP INFORMATION IS DESTROYED BY INSTR. 501-510      MAIN 150
C     ***** IF THE COMPUTER MEMORY AVAILABLE IS EXCEEDED BY THIS FEATUREMAIN 160
C     ***** SUBROUTINES LAP500, LAP700, LAP800, LAPDRW, LAPAB AND LAPCONMAIN 170
C     ***** MAY BE REMOVED AND REPLACED BY THE FOLLOWING 4 DUMMIES      MAIN 180
C     SUBROUTINE LAP500(NTYPE)                                          MAIN 190
C     RETURN                                                            MAIN 200
C     END                                                               MAIN 210
C     SUBROUTINE LAP700(NA,ICQ)                                         MAIN 220
C     RETURN                                                            MAIN 230
C     END                                                               MAIN 240
C     SUBROUTINE LAP800(NA1,NA2,ICQ)                                    MAIN 250
C     RETURN                                                            MAIN 260
C     END                                                               MAIN 270
C     SUBROUTINE LAPDRW(Y,NPEN,NCQ)                                     MAIN 280
C     RETURN                                                            MAIN 290
C     END                                                               MAIN 300
      REAL*8 CHEM                                                       MAIN 310
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    MAIN 320
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)MAIN 330
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) MAIN 340
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) MAIN 350
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   MAIN 360
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   MAIN 370
      DIMENSION XLNG(3),XO(3),XT(3)                                     MAIN 380
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   MAIN 390
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD MAIN 400
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1MAIN 410
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   MAIN 420
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                MAIN 430
      LTNO=0                                                            MAIN 440
    2 CALL PRIME                                                        MAIN 450
C     ***** READ JOB TITLE CARD *****                                   MAIN 460
      READ (IN,4)(TITLE(I),I=1,18)                                      MAIN 470
    4 FORMAT(18A4)                                                      MAIN 480
      WRITE (NOUT,6)(TITLE(I),I=1,18)                                   MAIN 490
    5 FORMAT(1H010X,18A4)                                               MAIN 500
    6 FORMAT(1H110X,18A4)                                               MAIN 510
      CALL PRELIM                                                       MAIN 520
      WRITE (NOUT,6)(TITLE(I),I=1,18)                                   MAIN 530
      ISAVE=0                                                           MAIN 540
      GO TO 507                                                         MAIN 550
    7 ISAVE=0                                                           MAIN 560
C     ***** ZERO AIN ARRAY *****                                        MAIN 570
    8 DO 10 J=1,140                                                     MAIN 580
   10 AIN(J)=0.                                                         MAIN 590
   11 FORMAT(1H04X,17H(((((( INSTRUCTIONI5,6H )))))))                   MAIN 600
   12 FORMAT(I3,I6,7F9.0)                                               MAIN 610
   13 FORMAT(I3,I6,7E15.8)                                              MAIN 620
   14 FORMAT(1H 9X,7E15.7)                                              MAIN 630
C     ***** READ NEW INSTRUCTION CARD *****                             MAIN 640
      NCD=0                                                             MAIN 650
      N1=-6                                                             MAIN 660
   16 N1=N1+7                                                           MAIN 670
      N2=N1+6                                                           MAIN 680
      IF(ISAVE)22,18,18                                                 MAIN 690
   18 READ (IN,12)IC,NF,(AIN(I),I=N1,N2)                                MAIN 700
      IF(ISAVE)24,24,20                                                 MAIN 710
   20 WRITE (NSR)IC,NF,(AIN(I),I=N1,N2)                                 MAIN 720
      GO TO 24                                                          MAIN 730
   22 READ (NSR)IC,NF,(AIN(I),I=N1,N2)                                  MAIN 740
      IF(IC)7,24,24                                                     MAIN 750
   24 IF(N1-1)26,26,30                                                  MAIN 760
   26 WRITE (NOUT,11)NF                                                 MAIN 770
      NF1=NF                                                            MAIN 780
      IF(NF1)28,8,30                                                    MAIN 790
   28 IF(NF1+2)2,2,3000                                                 MAIN 800
   30 WRITE (NOUT,14)(AIN(I),I=N1,N2)                                   MAIN 810
   32 IC=IC+1                                                           MAIN 820
      GO TO (90,16,38,50),IC                                            MAIN 830
   33 FORMAT(I3,6X,5I3,8F6.0)                                           MAIN 840
   34 FORMAT(6I3,8E12.5)                                                MAIN 850
   35 FORMAT(1H 11X,5I3,8F11.5)                                         MAIN 860
C     ***** READ FORMAT 2 TRAILER CARDS *****                           MAIN 870
   38 NCD=NCD+1                                                         MAIN 880
      IF(ISAVE)44,40,40                                                 MAIN 890
   40 READ (IN,33)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                MAIN 900
      IF(ISAVE)46,46,42                                                 MAIN 910
   42 WRITE (NSR)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                 MAIN 920
      GO TO 46                                                          MAIN 930
   44 READ (NSR)IC,(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                  MAIN 940
   46 WRITE (NOUT,35)(KD(I,NCD),I=1,5),(CD(I,NCD),I=1,8)                MAIN 950
      GO TO 32                                                          MAIN 960
C     ***** READ FORMAT 3 TRAILER CARD *****                            MAIN 970
   50 IF(ISAVE)52,54,54                                                 MAIN 980
   52 READ (NSR)(TITLE2(I),I=1,18)                                      MAIN 990
      GO TO 55                                                          MAIN1000
   54 READ (IN ,4)(TITLE2(I),I=1,18)                                    MAIN1010
   55 WRITE (NOUT,5)(TITLE2(I),I=1,18)                                  MAIN1020
      IF(ISAVE)90,90,56                                                 MAIN1030
   56 WRITE (NSR)(TITLE2(I),I=1,18)                                     MAIN1040
C     ***** EXECUTE INSTRUCTION *****                                   MAIN1050
   90 NJ=NF1/100                                                        MAIN1060
      NJ2=NF1-NJ*100                                                    MAIN1070
      NJ3=MOD(NJ2,10)                                                   MAIN1080
      IF(NJ-12)98,92,92                                                 MAIN1090
   92 CALL SPACE(NF1)                                                   MAIN1100
      IF(NG)94,8,94                                                     MAIN1110
   94 CALL ERPNT(0.,NF1)                                                MAIN1120
      GO TO 8                                                           MAIN1130
C     ******BRANCH TABLE FOR FUNCTION TYPES******                       MAIN1140
   98 GO TO(100,200,300,400,500,600,700,800,900,1000,1100),NJ           MAIN1150
C     *******STRUCTURE ANALYSIS FUNCTIONS*******                        MAIN1160
  100 GO TO (101,101,104,104,101,101,94),NJ2                            MAIN1170
  101 CALL SEARC                                                        MAIN1180
      GO TO 8                                                           MAIN1190
C     ***** ANISOTROPIC TEMP FACTOR OUTPUT *****                        MAIN1200
  104 DO 164 I=1,NATOM                                                  MAIN1210
      IF(MOD(I,14)-1)134,114,134                                        MAIN1220
  114 WRITE (NOUT,6)(TITLE(J),J=1,18)                                   MAIN1230
      WRITE (NOUT,129)                                                  MAIN1240
  129 FORMAT(1H010X,4HATOM3X,16HRMS DISPLACEMENT3X,31HROW VECTORS, BASEDMAIN1250
     1 ON REFERENCE17X,29HPROBABILITY COVARIANCE MATRIX)                MAIN1260
  134 T1=55501.+FLOAT(I)*100000.                                        MAIN1270
      CALL PAXES(T1,-3)                                                 MAIN1280
      IF(NG)144,154,144                                                 MAIN1290
  144 CALL ERPNT(T1,104)                                                MAIN1300
  149 FORMAT(1H010X,A6,F10.6,6X,3F12.7,10X,3F12.7)                      MAIN1310
  154 WRITE (NOUT,149)CHEM(I),RMS(1),(PAC(J,1),J=1,3),(Q(J,1)           MAIN1320
     1,J=1,3)                                                           MAIN1330
  164 WRITE (NOUT,159)(RMS(K),(PAC(J,K),J=1,3),(Q(J,K),J=1,3)           MAIN1340
     1,K=2,3)                                                           MAIN1350
  159 FORMAT(1H 16X,F10.6,6X,3F12.7,10X,3F12.7)                         MAIN1360
      GO TO 8                                                           MAIN1370
C     *******PLOTTER INITIALIZE,FRAME ADVANCE,TERMINATE FUNCTIONS*******MAIN1380
  200 CALL F200                                                         MAIN1390
      GO TO 8                                                           MAIN1400
  300 GO TO (301,302,303,94),NJ2                                        MAIN1410
C     *******PLOT DIMENSIONS*******                                     MAIN1420
  301 IF(AIN(1))321,321,311                                             MAIN1430
  311 XLNG(1)=AIN(1)                                                    MAIN1440
  321 IF(AIN(2))341,341,331                                             MAIN1450
  331 XLNG(2)=AIN(2)                                                    MAIN1460
  341 IF(AIN(3))361,351,351                                             MAIN1470
  351 VIEW=AIN(3)                                                       MAIN1480
  361 IF(AIN(4))381,381,371                                             MAIN1490
  371 BRDR=AIN(4)                                                       MAIN1500
  381 WRITE (NOUT,389)XLNG(1),XLNG(2),BRDR                              MAIN1510
  389 FORMAT(1H010X,11HPLOT LIMITSF6.2,3H BYF6.2,15H IN.  INCLUDINGF6.2,MAIN1520
     112H  IN. MARGIN)                                                  MAIN1530
  391 WRITE (NOUT,399)VIEW                                              MAIN1540
  399 FORMAT(1H 10X,13HVIEW DISTANCEF7.3,7H INCHES)                     MAIN1550
      GO TO 8                                                           MAIN1560
C     *******LEGEND ROTATION*******                                     MAIN1570
  302 THETA=AIN(1)                                                      MAIN1580
      T1=THETA*.01745329252                                             MAIN1590
      COSTH=COS(T1)                                                     MAIN1600
      SINTH=SIN(T1)                                                     MAIN1610
      DO 312 J=1,9                                                      MAIN1620
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  312 SYMB(J,1)=0.
      SYMB(1,1)=COSTH                                                   MAIN1630
      SYMB(2,2)=COSTH                                                   MAIN1640
      SYMB(3,3)=1.                                                      MAIN1650
      SYMB(2,1)=SINTH                                                   MAIN1660
      SYMB(1,2)=-SINTH                                                  MAIN1670
      WRITE (NOUT,319)THETA                                             MAIN1680
  319 FORMAT(1H010X,44HREGULAR TITLE AND SYMBOL ROTATION IN DEGREESF8.2) MAIN1690
      GO TO 8                                                           MAIN1700
C     ***** RETRACE DISPLACEMENT *****                                  MAIN1710
  303 DISP=AIN(1)                                                       MAIN1720
      WRITE (NOUT,313)DISP                                              MAIN1730
  313 FORMAT(1H010X,22HRETRACE DISPLACEMENT =F7.4,5H INCH)              MAIN1740
      GO TO 8                                                           MAIN1750
C     *******ATOM LIST FUNCTIONS*******                                 MAIN1760
  400 GO TO (401,401,401,401,401,401,490, 94, 94,410,                   MAIN1770
     1       401,401,401,401,401,401, 94),NJ2                           MAIN1780
  401 CALL F400                                                         MAIN1790
      GO TO 490                                                         MAIN1800
  410 LATM=0                                                            MAIN1810
      DO 420 I=1,500                                                    MAIN1820
      DO 420 J=1,4                                                      MAIN1830
  420 ATOMS(J,I)=0.                                                     MAIN1840
  490 IF(LATM)8,8,491                                                   MAIN1850
  491 WRITE (NOUT,499)(ATOMS(1,I),I=1,LATM)                             MAIN1860
  499 FORMAT(1H010X,23HCONTENTS OF ATOMS ABRAY/(15X,10F10.0))           MAIN1870
      GO TO 8                                                           MAIN1880
C     *******CARTESIAN COORDINATE SYSTEM FUNCTIONS*******               MAIN1890
  500 CALL F500                                                         MAIN1900
      WRITE  (NOUT,503)(ORGN(J),J=1,3)                                  MAIN1910
  503 FORMAT(1H0,10X,     44HORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.MAIN1930
     1,3F15.6)                                                          MAIN1940
      IF(NJ3-3)507,539,504                                              MAIN1950
  504 IF(NJ3-6)601,507,601                                              MAIN1955
  507 WRITE (NOUT,529)                                                  MAIN1960
      WRITE (NOUT,519)((REFV(J,I),I=1,3),(AAREV(J,I),I=1,3),J           MAIN1970
     1=1,3)                                                             MAIN1980
      GO TO 8                                                           MAIN1990
  509 FORMAT(1H010X, 49HORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXEMAIN2000
     1S18X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VECMAIN2010
     2TOR8X,8HZ VECTOR)                                                 MAIN2020
  519 FORMAT(1H 10X,3E16.7,8X,3E16.7)                                   MAIN2030
  529 FORMAT(1H010X,51HORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXMAIN2040
     1ES16X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VEMAIN2050
     2CTOR8X,8HZ VECTOR)                                                MAIN2060
  539 WRITE (NOUT,509)                                                  MAIN2070
      WRITE (NOUT,519)((WRKV(J,I),I=1,3),(AAWRK(J,I),I=1,3),J           MAIN2080
     1=1,3)                                                             MAIN2090
      GO TO 8                                                           MAIN2100
C     *******PLOT CENTERING FUNCTIONS*******                            MAIN2110
  600 CALL F600                                                         MAIN2120
  601 WRITE (NOUT,609)XO(1),XO(2),SCAL1,SCAL2                           MAIN2130
  609 FORMAT(1H010X,31HORIGIN POINT IN PLOTTER COORD.(F6.2,2H ,F6.2,8H ) MAIN2140
     1 IN.  / 11X,15HOVERALL SCALE =F6.3,32H INCH/ANGSTROM ELLIPSOID SCAMAIN2150
     2LE =F6.3)                                                         MAIN2160
      GO TO 391                                                         MAIN2170
C     *******ELLIPSOID AND SYMBOL PLOT FUNCTIONS*******                 MAIN2180
C     ********FILL OUT DETAILS FOR SPECIAL MODELS********               MAIN2190
  700 GO TO (701,702,704,705,709,94),NJ3                                MAIN2200
  701 AIN(3)=8.                                                         MAIN2210
      GO TO 703                                                         MAIN2220
  702 AIN(3)=0.                                                         MAIN2230
  703 AIN(1)=4.                                                         MAIN2240
      AIN(2)=0.                                                         MAIN2250
      AIN(4)=0.                                                         MAIN2260
      GO TO 709                                                         MAIN2270
  704 AIN(1)=3.                                                         MAIN2280
      AIN(2)=-5.                                                        MAIN2290
      GO TO 706                                                         MAIN2300
  705 AIN(1)=1.                                                         MAIN2310
      AIN(2)=0.                                                         MAIN2320
  706 AIN(3)=1.                                                         MAIN2330
      AIN(4)=5.                                                         MAIN2340
  709 CALL F700                                                         MAIN2350
      GO TO 8                                                           MAIN2360
C     *******BOND FUNCTIONS*******                                      MAIN2370
  800 CALL F800                                                         MAIN2380
      GO TO 8                                                           MAIN2390
C     *******TITLE FUNCTIONS*******                                     MAIN2400
  900 CALL F900                                                         MAIN2410
      GO TO 8                                                           MAIN2420
C     *******CELL OUTLINE FUNCTIONS*******                              MAIN2430
 1000 CALL F1000                                                        MAIN2440
      GO TO 8                                                           MAIN2450
C     *******SAVE SEQUENCE FUNCTIONS*******                             MAIN2460
 1100 IF(NJ2-2)1101,1102,1103                                           MAIN2470
 1101 ISAVE=1                                                           MAIN2480
      GO TO 1104                                                        MAIN2490
 1102 ISAVE=0                                                           MAIN2500
      J=-1                                                              MAIN2510
      END FILE NSR                                                      MAIN2520
      GO TO 1104                                                        MAIN2530
 1103 ISAVE=-1                                                          MAIN2540
 1104 REWIND NSR                                                        MAIN2550
      GO TO 8                                                           MAIN2560
C     ***** TERMINATE PLOTTER TAPE IF NECESSARY *****                  MAIN2570
 3000 IF(LTNO)3005,3010,3005                                            MAIN2580
 3005 AIN(1)=-.000001                                                   MAIN2590
      AIN(2)= 0.0                                                       MAIN2600
      NJ2=2                                                             MAIN2610
      CALL F200                                                         MAIN2620
 3010 CALL EXIT                                                         MAIN2630
      STOP                                                              MAIN2640
      END                                                               MAIN2650


      FUNCTION ARCCOS(X)
C     ARCCOS(X) IN DEGREES                                              ARCC  10
      IF(1.0-ABS(X))1,2,2                                               ARCC  20
    1 X=SIGN(1.0,X)                                                     ARCC  30
    2 IF(X)3,4,5                                                        ARCC  40
    3 ARCCOS=180.0+ATAN(SQRT(1.0-X*X)/X)*57.29577951                    ARCC  50
      GO TO 6                                                           ARCC  60
    4 ARCCOS=90.0                                                       ARCC  70
      GO TO 6                                                           ARCC  80
    5 ARCCOS=ATAN (SQRT(1.0-X*X)/X)*57.29577951                         ARCC  90
    6 RETURN                                                            ARCC 100
      END                                                               ARCC 110
                                                                        ARCC 120


      SUBROUTINE ATOM(QA,Z)
C     ATOM COORDINATE SUBROUTINE                                        ATOM  10
      DIMENSION X(3),Z(3)                                               ATOM  20
      REAL*8 CHEM                                                       ATOM  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ATOM  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) ATOM  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) ATOM  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ATOM  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   ATOM  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ATOM  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     ATOM 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ATOM 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ATOM 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1ATOM 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ATOM 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ATOM 150
      K=QA/100000.0                                                     ATOM 160
      IF(K)109,109,117                                                  ATOM 170
  109 X(1)=0.0                                                          ATOM 180
      X(2)=0.0                                                          ATOM 190
      X(3)=0.0                                                          ATOM 200
      GO TO 125                                                         ATOM 210
  117 IF(K-NATOM)119,119,503                                            ATOM 220
  503 NG=5                                                              ATOM 230
      GO TO 325                                                         ATOM 240
  119 DO 123 J=1,3                                                      ATOM 250
  123 X(J)=P(J,K)                                                       ATOM 260
  125 TA=ABS(QA)                                                        ATOM 270
      KSYM=AMOD(TA,100000.0)                                            ATOM 280
      KT=KSYM/100                                                       ATOM 290
      KS=KSYM-100*KT                                                    ATOM 300
      IF(KS-NSYM)203,203,403                                            ATOM 310
  403 NG=4                                                              ATOM 320
      GO TO 325                                                         ATOM 330
  203 IF(KS)403,205,213                                                 ATOM 340
  205 Z(1)=X(1)                                                         ATOM 350
      Z(2)=X(2)                                                         ATOM 360
      Z(3)=X(3)                                                         ATOM 370
      GO TO 311                                                         ATOM 380
  213 DO 223 K=1,3                                                      ATOM 390
      Z(K)=TS(K,KS)                                                     ATOM 400
      DO 223 J=1,3                                                      ATOM 410
  223 Z(K)=Z(K)+FS(J,K,KS)*X(J)                                         ATOM 420
  311 IF(KT)403,325,313                                                 ATOM 430
  313 IF(KT-555)317,315,317                                             ATOM 440
  315 KSYM=KS                                                           ATOM 450
      GO TO 325                                                         ATOM 460
  317 K1=KT/100                                                         ATOM 470
                                                                        ATOM 480
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      K=KT-100*K1                                                       ATOM 490
      K2=K/10                                                           ATOM 500
      K3=K-10*K2                                                        ATOM 510
      Z(1)=Z(1)+FLOAT(K1-5)                                             ATOM 520
      Z(2)=Z(2)+FLOAT(K2-5)                                             ATOM 530
      Z(3)=Z(3)+FLOAT(K3-5)                                             ATOM 540
  325 RETURN                                                            ATOM 550
      END                                                               ATOM 560

      SUBROUTINE AXEQB(A1,X,B1,JJJ)                                     AXEQ  10
C     ***** SOLUTION OF MATRIX EQUATION AX=B FOR X *****                AXEQ  20
C     ***** USES METHOD OF TRIANGULAR ELIMINATION *****                 AXEQ  30
C     ***** B AND X HAVE DIMENSIONS (3,JJJ),A IS ALWAYS (3,3)           AXEQ  40
C     ***** TO INVERT A MAKE B 3 BY 3 IDENITY MATRIX *****              AXEQ  50
      DIMENSION A1(3,3),A(3,3),B(3,3),B1(3,3),X(3,3)                    AXEQ  60
      NV=JJJ                                                            AXEQ  70
C     ***** TRANSFER DATA *****                                         AXEQ  80
      DO 2 I=1,3                                                        AXEQ  90
      DO 2 J=1,3                                                        AXEQ 100
      IF(NV-J) 2,1,1                                                    AXEQ 110
    1 B(I,J)=B1(I,J)                                                    AXEQ 120
    2 A(I,J)=A1(I,J)                                                    AXEQ 130
C     ***** TRIANGULARIZE MATRIX A *****                                AXEQ 140
      DO 17 I=1,2                                                       AXEQ 150
      S=0.0                                                             AXEQ 160
      DO 4 J=I,3                                                        AXEQ 170
      R=ABS(A(J,I))                                                     AXEQ 180
      IF(R-S)4,3,3                                                      AXEQ 190
    3 S=R                                                               AXEQ 200
      L=J                                                               AXEQ 210
    4 CONTINUE                                                          AXEQ 220
      IF(L-I)5,10,5                                                     AXEQ 230
    5 DO 6 J=I,3                                                        AXEQ 240
      S=A(I,J)                                                          AXEQ 250
      A(I,J)=A(L,J)                                                     AXEQ 260
    6 A(L,J)=S                                                          AXEQ 270
      DO 8 J=1,NV                                                       AXEQ 280
      S=B(I,J)                                                          AXEQ 290
      B(I,J)=B(L,J)                                                     AXEQ 300
    8 B(L,J)=S                                                          AXEQ 310
   10 TEM=A(I,I)                                                        AXEQ 320
      IF(TEM)11,17,11                                                   AXEQ 330
   11 IPO=I+1                                                           AXEQ 340
      DO 16 J=IPO,3                                                     AXEQ 350
      IF(A(J,I))12,16,12                                                AXEQ 360
   12 S=A(J,I)/TEM                                                      AXEQ 370
      A(J,I)=0.0                                                        AXEQ 380
      DO 13 K=IPO,3                                                     AXEQ 390
   13 A(J,K)=A(J,K)-A(I,K)*S                                            AXEQ 400
      DO 15 K=1,NV                                                      AXEQ 410
   15 B(J,K)=B(J,K)-B(I,K)*S                                            AXEQ 420
   16 CONTINUE                                                          AXEQ 430
   17 CONTINUE                                                          AXEQ 440
C     ***** MODIFY SINGULAR MATRIX *****                                AXEQ 450
      DO 20 I=1,3                                                       AXEQ 460
      IF(A(I,I))20,19,20                                                AXEQ 470
   19 A(I,I)=AMAX1(1.E-25,AMAX1(A(1,1),A(2,2),A(3,3))*1.E-15)           AXEQ 480
   20 CONTINUE                                                          AXEQ 490
      DO 24 K=1,NV                                                      AXEQ 500
      DO 24 I=1,3                                                       AXEQ 510
      N=4-I                                                             AXEQ 520
      M=N+1                                                             AXEQ 530
      TEM=B(N,K)                                                        AXEQ 540
      IF(3-M)23,21,21                                                   AXEQ 550
   21 DO 22 J=M,3                                                       AXEQ 560
   22 TEM=TEM-A(N,J)*B(J,K)                                             AXEQ 570
   23 B(N,K)=TEM/A(N,N)                                                 AXEQ 580
   24 X(N,K)=B(N,K)                                                     AXEQ 590
      RETURN                                                            AXEQ 600
      END                                                               AXEQ 610

      SUBROUTINE AXES(U,V,X,ITYPE)                                      AXES  10
C     ***** STORE THREE ORTHOGONAL VECTORS EACH 1 ANGSTROM LONG *****   AXES  20
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         AXES  30
C     *****IABS(ITYPE)=1 W(1)=U,W(2)=(UXV),W(3)=UX(UXV) *****           AXES  40
C     *****IABS(ITYPE)=2 W(1)=U,W(2)=(UXV)XU,W(3)=(UXV) *****           AXES  50
C     ***** ITYPE=0 W(1)=A,W(2)=(AXB)XA,W(3)=(AXB), ABC=CELL VECTORS ***AXES  60
      DIMENSION U(3),V(3),W(3,3),X(3,3)                                 AXES  70
      IT=ITYPE                                                          AXES  80
      IF(IT)115,105,115                                                 AXES  90
  105 U(1)=1.                                                           AXES 100
      U(2)=0.                                                           AXES 110
      U(3)=0.                                                           AXES 120
      V(1)=0.                                                           AXES 130
      V(2)=1.                                                           AXES 140
      V(3)=0.                                                           AXES 150
  115 DO 125 J=1,3                                                      AXES 160
  125 W(J,1)=U(J)                                                       AXES 170
      IF(IABS(IT)-1)145,135,145                                         AXES 180
  135 CALL NORM(U,V,W(1,2),IT)                                          AXES 190
      CALL NORM(U,W(1,2),W(1,3),IT)                                     AXES 200
      GO TO 155                                                         AXES 210
  145 CALL NORM(U,V,W(1,3),IT)                                          AXES 220
      CALL NORM(W(1,3),U,W(1,2),IT)                                     AXES 230
  155 DO 195 I=1,3                                                      AXES 240
      IF(IT)165,165,175                                                 AXES 250
  165 IC=-1                                                             AXES 260
      GO TO 195                                                         AXES 270
  175 IC=1                                                              AXES 280
  195 CALL UNIT(W(1,I),X(1,I),IC)                                       AXES 290
      RETURN                                                            AXES 300
      END                                                               AXES 310

      SUBROUTINE BOND(Z1,Z2,NB,NA1,NA2)                                 BOND  10
      DIMENSION B(3,3),E(3,3),S(3,3),U(3,3),VUE(3)                      BOND  20
      DIMENSION V7(3),W(13,2),X(3),Z(3)                                 BOND  30
      REAL*8 CHEM                                                       BOND  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    BOND  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) BOND  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) BOND  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) BOND  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   BOND  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   BOND 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     BOND 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   BOND 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD BOND 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1BOND 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   BOND 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                BOND 160
C     ***** OBTAIN POSITIONAL PARAMETERS *****                          BOND 170
      NG1=0                                                             BOND 180
      DO 105 J=1,26                                                     BOND 190
  105 W(J,1)=0.                                                         BOND 200
      W(1,1)=Z1                                                         BOND 210
      W(1,2)=Z2                                                         BOND 220
      DO 135 I=1,2                                                      BOND 230
      CALL XYZ(W(1,I),W(4,I),2)                                         BOND 240
      IF(NG)125,110,125                                                 BOND 250
  110 DO 115 J=1,3                                                      BOND 260
  115 W(J+6,I)=XT(J)                                                    BOND 270
      K=W(1,I)/100000.                                                  BOND 280
      L=W(1,I)-FLOAT(K)*100000.                                         BOND 290
      CALL PLTXY(W(4,I),W(2,I))                                         BOND 300
      IF(EDGE-BRDR*.25)120,128,128                                      BOND 310
  120 NG=10                                                             BOND 320
  125 NG1=1                                                             BOND 330
      WRITE (NOUT,136)CHEM(K),K,L,(W(J,I),J=2,9)                        BOND 340
      CALL ERPNT(W(1,I),800)                                            BOND 350
      GO TO 135                                                         BOND 360
  128 IF(NJ2-10)130,135,135                                             BOND 370
  130 WRITE (NOUT,136)CHEM(K),K,L,(W(J,I),J=2,9)                        BOND 380
  135 CONTINUE                                                          BOND 390
  136 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)   2F8.2,5X,3F8.3,13X,3F8.4)    BOND 400
      IF(NG1)999,140,999                                                BOND 410
  140 CALL DIFV(W(7,1),W(7,2),V7)                                       BOND 420
      DIST=SQRT(VMV(V7,AA,V7))                                          BOND 430
      IF(MOD(NJ2,10)-3)143,142,142                                      BOND 440
  142 HGT=SCL*.12                                                       BOND 450
      CALL SIMBOL(W(2,1),W(3,1),HGT,MOD(IFIX(W(1,1)/100000.),10),0.,-   BOND 460
     11)                                                                BOND 470
      CALL SIMBOL(W(2,2),W(3,2),HGT,MOD(IFIX(W(1,2)/100000.),10),0.,-   BOND 480
     12)                                                                BOND 490
      GO TO 570                                                         BOND 500
  143 KODE=KD(5,NB)                                                     BOND 510
      IF(KODE)145,144,146                                               BOND 520
  144 NBND=0                                                            BOND 530
      GO TO 148                                                         BOND 540
  145 KODE=-KODE                                                        BOND 550
  146 NBND=128/2**KODE                                                  BOND 560
C     ***** FIND UPPERMOST ATOM PUT IN POSITION ONE *****               BOND 570
  148 IF(VIEW)152,150,152                                               BOND 580
  150 W(12,1)=1.                                                        BOND 590
      W(12,2)=1.                                                        BOND 600
```

```
      IF(W(6,1)-W(6,2)) 165,175,175
C     *****VECTOR FROM ATOM TO VIEWPOINT *****
  152 DO 160 I=1,2
      DO 155 J=10,12
  155 W(J,I)=-W(J-6,I)
      W(12,I)=W(12,I)+VIEW
C     ***** DISTANCE SQUARED TO VIEWPOINT *****
  160 W(13,I)=VV(W(10,I),W(10,I))
      IF(W(13,2)-W(13,1)) 165,175,175
C     ***** SWITCH ATOMS *****
  165 DO 170 J=1,13
      T1=W(J,1)
      W(J,1)=W(J,2)
  170 W(J,2)=T1
C     ***** FORM IDEMFACTOR MATRIX *****
  175 DO 180 J=1,3
      E(J,J)=1.
      E(J+1,1)=0.
  180 E(J+5,1)=0.
C     ***** FORM VECTOR SET RADIAL TO BOND *****
      CALL DIPV(W(4,2),W(4,1),DA(1,3))
      CALL UNIT(DA(1,3),V3,1)
C     ***** UNIT VECTOR FROM BOND MIDPOINT TO REFERENCE VIEWPOINT *****
      DO 183 I=1,3
      V2(I)=0.0
      DO 181 J=1,3
  181 V2(I)=V2(I)+AABEV(J,3)*WRKV(J,I)
      IF(VIEW) 183,183,182
  182 V2(I)=V2(I)*VIEW-0.5*(W(I+3,1)+W(I+3,2))
  183 CONTINUE
      CALL UNIT(V2,V2,1)
      T6=ABS(VV(V3,V2))
      IF(.9994-T6) 185,185,187
C     ***** ALTERNATE CALC IF BOND IS ALONG REFERENCE VIEW DIRECTION ***
  185 DO 186 J=1,3
  186 V2(J)=W(J+9,1)+W(J+9,2)
      CALL UNIT(V2,V2,1)
      T6=ABS(VV(V3,V2))
      IF(.9994-T6) 390,390,187
  187 CALL AXES(V3,V2,B,1)
  188 T1=CD(3,NB)/SCAL2
      DO 190 J=1,3
      DA(J,1)=-B(J,2)*T1
  190 DA(J,2)=-B(J,3)*T1
      IF(NBND) 500,500,195
  195 CALL RADIAL(3)
C     ***** DERIVE QUADRICS FOR EACH ATOM *****
      DO 380 II=1,2
      CALL PAXES(W(1,II),2)
      IF(NG) 205,210,205
  205 CALL ERPNT(W(1,II),800)
      GO TO 999
C     ***** DOES BOND GO TO ELLIPSOID OR TO ENVELOPE *****
  210 T1=3-II*2
      DO 212 J=1,3
      V3(J)=V3(J)*T1
  212 VUE(J)=0.
      IF(KD(5,NB)) 260,260,215
  215 IF(VMV(V3,Q,W(10,II))) 220,260,260
  220 IBND=0
      IF(VIEW) 240,240,225
C     ***** DERIVE TANGENT CONE DIRECTLY WITHOUT ROTATING COORDINATES **
  225 T2=-(SCAL2*RMS(1)*RMS(2)*RMS(3))**2
      DO 230 J=1,3
      V1(J)=-W(J+9,II)/SCAL1
      VUE(J)=V1(J)/SCAL2
C     ***** INVERT ELLIPSOID MATRIX *****
      DO 230 K=J,3
      T1=0.0
      DO 228 I=1,3
  228 T1=T1+PAC(J,I)*PAC(K,I)*RMS(I)**2
      U(J,K)=T1
  230 U(K,J)=T1
C     *****  ADD POLARIZED COFACTOR MATRIX TO ELLIPSOID MATRIX *****
      DO 235 J=1,3
      J1=MOD(J,3)+1
      VJ1=V1(J1)
      J2=MOD(J+1,3)+1
      VJ2=V1(J2)
      DO 235 K=J,3
      K1=MOD(K,3)+1
      K2=MOD(K+1,3)+1
      S(J,K)=T2*Q(J,K)+(VJ2*(U(J1,K1)*V1(K2)-U(J1,K2)*V1(K1))
     1                 + VJ1*(U(J2,K2)*V1(K1)-U(J2,K1)*V1(K2)))
  235 S(K,J)=S(J,K)
      T5=0.0
      GO TO 300
C     ***** DERIVE TANGENT CYLINDER WITH AXIS ALONG Z *****
  240 T1=-1.0/Q(3,3)
      DO 250 J=1,2
      DO 245 K=1,2
  245 S(K,J)=Q(K,J)+Q(K,3)*Q(J,3)*T1
      S(3,J)=0.0
  250 S(J,3)=0.0
      S(3,3)=0.0
      GO TO 270
C     ***** TRANSFER ELLIPSOID *****
  260 DO 265 J=1,9
  265 S(J,1)=Q(J,1)
      IBND=II
  270 T5=1.
C     ***** CHECK FOR BOND TAPER *****
  300 IF(II-2) 305,310,310
  305 RADIUS=1.+T6*TAPER
      GO TO 320
  310 RADIUS=1.-T6*TAPER
  320 CALL MV(S,V3,V4)
      T2=VV(V3,V4)
C     ***** COMPUTE BOND INTERSECTION *****
      KL=5-II-II
      KSTP=4
      IF(NJ2-21) 324,322,322
  322 KSTP=32
  324 DO 335 K=1,65,KSTP
      DO 325 J=1,3
      V6(J)=D(J,K)*RADIUS
  325 V5(J)=V6(J)+VUE(J)
      T3=VV(V5,V4)
      T4=T3*T3-T2*(VMV(V5,S,V5)-T5)
      IF(T4) 345,330,330
  330 T4=SQRT(T4)
      T1=(T4-T3)/T2
      T3=(-T4-T3)/T2
      L=K+KL-1
      DO 335 J=1,3
      D(J,L)=(V6(J)+T1*V3(J))*SCL
  335 D(J,L+1)=(-V6(J)-T3*V3(J))*SCL
      IF(IBND+21-NJ2) 360,338,360
  338 IF(KD(5,NB)) 360,360,340
C     ***** FOR OVERLAP, MAKE BOND QUADRANGLE TANGENT TO ENVELOPING CONE
  340 T3=VV(VUE,V4)
      T4=T3**2-T2*(VMV(VUE,S,VUE)-T5)
      IF(T4) 345,350,350
  345 NG=13
      CALL ERPNT(W(1,II),800)
      GO TO 999
  350 T1=(SQRT(T4)-T3)/T2
      DO 355 J=1,3
      T4=(T1*V3(J)*SCL-0.5*(D(J,KL)+D(J,KL+64)))*1.001
      D(J,KL)=D(J,KL)+T4
  355 D(J,KL+64)=D(J,KL+64)+T4
  360 CALL PROJ(D(1,KL),DP(1,II),W(4,II),XO,VIEW,1,65,KSTP)
      IF(IBND-1) 370,365,370
  365 CALL PROJ(D(1,KL+5),DP(1,II+68),W(4,II),XO,VIEW,1,61,KSTP)
      GO TO 380
C     ***** RETRACE TOP HALF *****
  370 DO 375 K=4,64,4
      L=K+II
      M=L+64
      N=66-L
      DP(1,M)=DP(1,N)
  375 DP(2,M)=DP(2,N)
  380 CONTINUE
C     ***** CHECK FOR OVERLAP OR HIDDEN BOND *****
      DO 395 K=1,65,32
      T1=0.
      T2=0.
      DO 385 J=1,2
      T1=T1+(DP(J,K)-W(J+1,1))**2
  385 T2=T2+(DP(J,K+1)-W(J+1,1))**2
      IF(T2-T1) 390,390,395
  390 NG=14
      CALL ERPNT(W(1,2),800)
      GO TO 999
  395 CONTINUE
C     ***** CALL OVERLAP ROUTINE *****
      ICQ=0
      CALL LAP800(NA1,NA2,ICQ)
```

```
      IF (NJ2-21) 400,999,999
  400 IF (ICQ) 390,405,405
C     ***** DRAW BOND OUTLINE *****
  405 CALL DRAW(DP(1,1),0.,0.,3)
      DO 415 K=5,129,4
  415 CALL DRAW(DP(1,K),0.,0.,2)
      DO 420 K=2,66,4
  420 CALL DRAW(DP(1,K),0.,0.,2)
      CALL DRAW(DP(1,65),0.,0.,2)
C     ***** DRAW BOND DETAIL *****
  425 K=65
  430 K=K-NBND
      IF (K-1) 500,500,435
  435 CALL DRAW(DP(1,K),0.,0.,3)
      CALL DRAW(DP(1,K+1),0.,0.,2)
      K=K-NBND
      IF (K-1) 500,500,440
  440 CALL DRAW(DP(1,K+1),0.,0.,3)
      CALL DRAW(DP(1,K),0.,0.,2)
      GO TO 430
  500 HGT=CD(4,NB)
      OFF=CD(5,NB)
      IF (HGT) 570,570,510
C     ***** PERSPECTIVE BOND LABEL ROUTINE *****
C     ***** BASE DECISIONS ON REFERENCE SYSTEM *****
  510 K=0
      CALL DIFV(W(7,2),W(7,1),V7)
      CALL VM(V7,AAREV,V1)
      CALL AXES(V1,E(1,3),U,1)
      DO 535 I=1,3
      T1=1.
      IF (I-2) 515,515,520
  515 IF (VV(U(1,I),SYMB(1,I))) 525,530,530
  520 IF (MOD(K,2)) 530,525,530
  525 T1=-1.
      K=K+1
  530 DO 535 J=1,3
      U(J,I)=U(J,I)*T1
  535 VT(J,I)=B(J,I)*T1
      DO 540 J=1,3
  540 VT(J,4)=.5*(W(J+3,1)+W(J+3,2))
C     ***** CHECK FOR EXCESS FORESHORTENING *****
      IF (FORE-ABS(U(3,1))) 545,550,550
  545 CALL NORM(U(1,2),SYMB(1,3),VT(1,1),1)
      VT(1,3)=SYMB(1,3)
      VT(2,3)=SYMB(2,3)
      VT(3,3)=SYMB(3,3)
      HGT=CD(6,NB)
      OFF=CD(7,NB)
      IF (HGT) 550,999,550
  550 T1=CD(8,NB)
      Z(1)=VT(1,4)-HGT*(11.+3.*T1)/7.
      Z(2)=VT(2,4)+OFF-HGT*.5
      Z(3)=VT(3,4)
      XO(3)=Z(3)
      ITILT=1
      I9=T1+2.
      T9=10.**I9
      DISTR=AINT((DIST*T9)+0.5)/T9 +.0001
      CALL NUMBUR(Z(1),Z(2),HGT,DISTR,0.,I9)
  570 ITILT=0
      IF (NJ2-10) 580,999,999
  580 WRITE (NOUT,571) DIST
  571 FORMAT(1H 59X,10HDISTANCE =F8.3/1H )
  999 RETURN
      END
```

```
      SUBROUTINE DIFV(X,Y,Z)
C     VECTOR - VECTOR
C     Z(3)=X(3)-Y(3)
      DIMENSIONX(3),Y(3),Z(3)
      DO 111 I=1,3
  111 Z(I)=X(I)-Y(I)
      RETURN
      END
```

```
      SUBROUTINE DRAW(W,DX,DY,NPEN)
      DIMENSION W(3),X(3),Y(3),Z(3)
      REAL*8 CHEM
      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(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),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,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      Y(1)=W(1)+DX
      Y(2)=W(2)+DY
      IF (ITILT) 115,140,115
C     ***** ROTATE FOR PERSPECTIVE TITLE *****
  115 Y(3)=XO(3)
      DO 120 I=1,3
  120 Z(I)=Y(I)-VT(I,4)
      DO 130 I=1,3
  130 X(I)=VT(I,1)*Z(1)+VT(I,2)*Z(2)+VT(I,3)*Z(3)+VT(I,4)
      CALL PLTXY(X,Y)
C     ***** CHECK BOUNDRY *****
  140 DO 160 J=1,2
      IF (Y(J)-XLNG(J)+.1) 150,150,145
  145 Y(J)=XLNG(J)-.1
  150 IF (Y(J)-.1) 155,160,160
  155 Y(J)=.1
  160 CONTINUE
C     ***** CHECK FOR OVERLAP *****
      NCQ=0
      CALL LAPDRW(Y,NPEN,NCQ)
      IF (NCQ) 165,165,170
C     ***** CALL PLOTTING ROUTINE IF NO OVERLAPPING ELEMENTS ARE STORED
  165 CALL SCRIBE(Y,NPEN,LTNO)
  170 RETURN
      END
```

```
      SUBROUTINE EIGEN (W,VALU,VECT)
C     ***** EIGENVALUES AND EIGENVECTORS OF 3X3 MATRIX *****
      DIMENSION W(3,3),VALU(3),VECT(3,3),A(3,3),B(3,3),V(3),U(3)
      COMMON NG
C     ***** STATEMENT FUNCTION *****
      PHIF(Z)=((B2-Z)*Z+B1)*Z+B0
C     ***** START OF PROGRAM *****
      ERRND=5.E-7
      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=SQRT(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)
     1+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)-
     1A(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=ABS(VOLD-VNEW)
      IF (TEM-ERRND) 250,250,205
  205 IF (VOLD) 210,225,210
```

```
  210 IF (ABS(TEM/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(TEM) 255,265,260
C     ***** IGNORE IMAGINARY COMPONENT OF COMPLEX ROOT *****
  255 TEM=0.
      GO TO 265
  260 TEM=SQRT(TEM)
  265 U(1)=.5*(C1-TEM)
      U(2)=.5*(C1+TEM)
C     ***** SORT ROOTS *****
      DO 275 J=1,2
      IF(U(J)-U(3)) 275,275,270
  270 TEM=U(J)
      U(J)=U(3)
      U(3)=TEM
  275 CONTINUE
      LLL=-2
      DO 375 III=1,2
C     ***** CHECK FOR MULTIPLE ROOTS *****
      TEM=ERRND*100.
      NG=0
      L=1
      DO 305 I=1,2
      IF(U(I+1)-U(I)-TEM) 300,300,290
  290 IF(U(I)) 295,305,295
  295 IF(ABS((U(I+1)-U(I))/U(I))-TEM) 300,300,305
  300 L=L-1
      NG=NG-2*I
  305 CONTINUE
      IF(LLL-L) 308,400,400
  308 LLL=L
C     ***** EIGENVECTOR ROUTINE *****
      DO 375 II=1,3
      T1=U(II)
      IF(L) 315,310,322
C     ***** TWO VECTORS NULL FOR DOUBLE ROOT *****
  310 IF(NG+5-II) 315,322,315
C     ***** ALL VECTORS NULL FOR TRIPLE ROOT *****
  315 DO 320 J=1,3
  320 VECT(J,II)=0.0
      GO TO 375
  322 DO 325 J=1,3
  325 A(J,J)=W(J,J)-T1
      SMAX=0.0
      DO 355 I=1,3
      I1=1
      IF(I-2) 335,335,340
  335 I1=I+1
  340 B(I,1)=A(I,2)*A(I1,3)-A(I,3)*A(I1,2)
      B(I,2)=A(I,3)*A(I1,1)-A(I,1)*A(I1,3)
      B(I,3)=A(I,1)*A(I1,2)-A(I,2)*A(I1,1)
      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 CONTINUE
      IF(SMAX) 353,353,360
  353 NG=7
      GO TO 375
  360 SMAX=SQRT(SMAX)
      DO 365 J=1,3
  365 V(J)=B(IMAX,J)/SMAX
C     ***** REFINE EIGENVECTOR *****
      CALL AXEQB(A,V,V,1)
      TEM=AMAX1(ABS(V(1)),ABS(V(2)),ABS(V(3)))
      DO 370 J=1,3
  370 V(J)=V(J)/TEM
      CALL UNIT(V,VECT(1,II),1)
C     ***** REFINE EIGENVALUE *****
      T1=VMV(VECT(1,II),W,VECT(1,II))
      U(II)=T1
  375 VALU(II)=T1
  400 RETURN
      END
```

```
EIGE 490
EIGE 500
EIGE 510
EIGE 520
EIGE 530
EIGE 540
EIGE 550
EIGE 560
EIGE 570
EIGE 580
EIGE 590
EIGE 600
EIGE 610
EIGE 620
EIGE 630
EIGE 640
EIGE 650
EIGE 660
EIGE 670
EIGE 680
EIGE 690
EIGE 700
EIGE 710
EIGE 720
EIGE 730
EIGE 740
EIGE 750
EIGE 760
EIGE 770
EIGE 780
EIGE 790
EIGE 800
EIGE 810
EIGE 820
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EIGE 970
EIGE 980
EIGE 990
EIGE1000
EIGE1010
EIGE1020
EIGE1030
EIGE1040
EIGE1050
EIGE1060
EIGE1070
EIGE1080
EIGE1090
EIGE1100
EIGE1110
EIGE1120
EIGE1130
EIGE1140
EIGE1150
EIGE1160
EIGE1170
EIGE1180
EIGE1190
EIGE1200
EIGE1210
EIGE1220
EIGE1230
EIGE1240
EIGE1250
EIGE1260
EIGE1270
EIGE1280
EIGE1290
EIGE1300
EIGE1310
EIGE1320
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      SUBROUTINE ERPNT(T1,N)                                            ERPN  10
      REAL*8 CHEM                                                       ERPN  20
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ERPN  30
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) ERPN  40
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) ERPN  50
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ERPN  60
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   ERPN  70
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ERPN  80
      DIMENSION XLNG(3),XO(3),XT(3)                                     ERPN  90
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ERPN 100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ERPN 110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1ERPN 120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ERPN 130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ERPN 140
      WRITE (NOUT,115)NG,T1,N                                           ERPN 150
  115 FORMAT(1H 10X,10HFAULT NG =I3,F10.0,I6/1H )                       ERPN 160
      NG=0                                                              ERPN 170
      RETURN                                                            ERPN 180
      END                                                               ERPN 190


      SUBROUTINE F200                                                   F200  10
      DIMENSION HEADER(4),PLA(3000)                                     F200  20
      DATA HEADER/3*4H    ,4H$   /,ZERO/0.0/                             F200  30
      REAL*8 CHEM                                                       F200  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F200  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F200  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F200  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F200  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F200  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F200 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F200 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F200 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F200 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F200 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F200 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F200 160
C     ***** CALCOMP CONTROL *****                                       F200 170
      NJQ = NJ2+1                                                       F200 180
      GO TO(260,200,225,205,210,260),NJQ                                F200 190
C     ***** INITIATE MECHANICAL CALCOMP PLOTTER (201 INSTRUCTION) ***** F200 200
  200 LTNO = 15                                                         F200 210
      CALL PLOTS(PLA,3000,LTNO)                                         F200 220
      GO TO 260                                                         F200 230
C     ***** INITIATE C.R.T. CALCOMP PLOTTER (203 INSTRUCTION) *****     F200 240
  205 LTNO = -99                                                        F200 250
      CALL JOBNUM(HEADER(1))                                            F200 260
      CALL IDAY(HEADER(2))                                              F200 270
      CALL CRT(PLA,3000,HEADER,0)                                       F200 280
C     ***** SET C.R.T. X,Y ORIGIN AND BEAM INTENSITY BASELINE *****     F200 290
      IZ = AIN(3)                                                       F200 300
      CALL CRT(AIN(1),AIN(2),IZ,3)                                      F200 310
      GO TO 215                                                         F200 320
C     ***** RESET BEAM INTENSITY (204 INSTRUCTION) *****                F200 330
  210 IZ = AIN(1)                                                       F200 340
      IF(IZ) 215,215,220                                                F200 350
  215 IZ = 18                                                           F200 360
  220 CALL CRT(ZERO,ZERO,IZ,7)                                          F200 370
      GO TO 260                                                         F200 380
C     ***** TERMINATE THE PLOT AND ADVANCE PLOTTER (202 INSTRUCTION) ***F200 390
  225 IF(LTNO) 235,260,230                                              F200 400
  230 CALL PLOT(AIN(1),AIN(2),-3)                                       F200 410
      GO TO 260                                                         F200 420
C     ***** THE FOLLOWING ARE FOR CRT FILM ADVANCE ETC. *****           F200 430
  235 IF(AIN(1)) 245,240,250                                            F200 440
C     ***** ADD BLOCK ADDRESS BUT DO NOT ADVANCE CRT FILM *****         F200 450
  240 IB = 1000                                                         F200 460
      GO TO 255                                                         F200 470
C     ***** ADVANCE CRT FILM AND CLOSE OUTPUT TAPE FILE ****            F200 480
  245 IB = 9000                                                         F200 490
      GO TO 255                                                         F200 500
C     ***** ADD BLOCK ADDRESS AND ADVANCE CRT FILM *****                F200 510
  250 IB = 0000                                                         F200 520
C     ***** IDENTIFICATION TITLE FRAME BETWEEN PLOTS *****              F200 530
      CALL CRT(ZERO,ZERO,IB,2)                                          F200 540
      CALL SIMBOL(0.2,0.0,0.25,TITLE(1),40.,72)                         F200 550
  255 CALL CRT(ZERO,ZERO,IB,2)                                          F200 560
  260 RETURN                                                            F200 570
      END                                                               F200 580


      SUBROUTINE F400                                                   F400  10
C     ***** ATOM LIST FUNCTIONS *****                                   F400  20
      REAL*8 CHEM                                                       F400  30
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      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(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),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,LTNC,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      NG=0
      IF(LATM)402,402,400
  400 DO 401 I=1,LATM
  401 CALL ATOM(ATOMS(1,I),ATOMS(2,I))
  402 IF(MOD(NJ2,10)-1)499,404,403
  403 CALL SEARC
      GO TO 499
C     ***** STORES (401) OR REMOVES (411) RUNS OF ATOMS *****
C     ***** RUN HIERARCHY = ATOM NO./SYM/ A/B/C TRANS. *****
  404 II=1
C     ***** FIND RUNS IN AIN ARRAY *****
  405 T1=AIN(II)
      IF(T1)410,410,420
  410 II=II+1
      IF(140-II)499,405,405
  420 JJ=II
C     ***** SET INITIAL RUN VALUES *****
      M1=T1/100000.
      M2=AMOD(T1,100.)
      M5=AMOD(T1/100.,1000.)
      IF(M5)422,422,423
  422 M5=555
  423 M3=M5/100
      M4=MOD(M5/10,10)
      M5=MOD(M5,10)
  425 JJ=JJ+1
      IF(140-JJ)435,430,430
  430 T2=-AIN(JJ)
      IF(T2)435,425,440
  435 II=JJ-1
C     ***** SET TERMINAL VALUES FOR DEGENERATE RUN *****
      N1=M1
      N2=M2
      N3=M3
      N4=M4
      N5=M5
      GO TO 450
  440 II=JJ
C     ***** SET TERMINAL RUN VALUES *****
      N1=T2/100000.
      N2=AMOD(T2,100.)
      N5=AMOD(T2/100.,1000.)
      IF(N5)445,445,446
  445 N5=555
  446 N3=N5/100
      N4=MOD(N5/10,10)
      N5=MOD(N5,10)
C     ***** LOOP THROUGH ALL RUNS *****
  450 DO 490 L5=M5,N5
      DO 490 L4=M4,N4
      DO 490 L3=M3,N3
      DO 490 L2=M2,N2
      DO 490 L1=M1,N1
      V1(1)=FLOAT(L1)*100000.+FLOAT(L3*10000+L4*1000+L5*100+I2)
      CALL ATOM(V1(1),V1(2))
      IF(NG)455,458,455
  455 CALL ERPNT(V1(1),401)
      GO TO 490
  458 CALL STOR
  490 CONTINUE
      GO TO 410
  499 RETURN
      END


      SUBROUTINE F500
      DIMENSION RM(3,3),V(3,4)
      REAL*8 CHEM
      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(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),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,LTNC,NATOM,NCD
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      NG=0
      IF(NJ2-11)500,700,710
  500 IF(NJ2-1)710,501,510
  501 T1=AIN(1)
      CALL ATOM(T1,ORGN)
      IF(NG)502,504,502
  502 CALL ERPNT(T1,501)
      CALL EXIT
  504 DO 506 K=1,4
      T1=AIN(K+1)
      CALL ATOM(T1,V(1,K))
      IF(NG)502,506,502
  506 CONTINUE
      DO 507 J=1,3
      V1(J)=V(J,2)-V(J,1)
  507 V2(J)=V(J,4)-V(J,3)
      IND=-1
      IF(AIN(7))509,509,508
  508 IND=-2
  509 CALL AXES(V1,V2,REFV,IND)
      GO TO 670
  510 IF(NJ2-4)515,511,599
C     ***** SHIFT ORIGIN FOR PROJECTION AXIS (IN INCHES) *****
  511 DO 513 J=1,3
      DO 512 K=1,3
  512 ORGN(J)=ORGN(J)+REFV(J,K)*AIN(K)/SCAL1
  513 XO(J)=XO(J)+AIN(J)
      GO TO 675
C     ***** FORM ROTATION MATRIX *****
  515 DO 552 L=1,139,2
      I=AIN(L)
      IF(I) 532,552,516
  516 X=AIN(L+1)*1.7453293E-2
      T1=COS(X)
      T2=SIN(X)
      I3=MOD(I+2,3)+1
      I1=MOD(I3,3)+1
      I2=MOD(I1,3)+1
      RM(I1,I1)=T1
      RM(I1,I2)=T2
      RM(I1,I3)=0.0
      RM(I2,I1)=-T2
      RM(I2,I2)=T1
      RM(I2,I3)=0.0
      RM(I3,I1)=0.0
      RM(I3,I2)=0.0
      RM(I3,I3)=1.0
      CALL MM(REFV,RM,V)
      IF(NJ2-3)518,525,599
  518 DO 522 J=1,3
      DO 522 I=1,3
  522 REFV(I,J)=V(I,J)
      GO TO 552
  525 DO 528 J=1,3
      DO 528 I=1,3
  528 WRKV(I,J)=V(I,J)
      GO TO 552
  532 IF(NJ2-3)535,552,599
  535 I=MOD(-I,3)
      DO 542 J=1,I
      DO 542 K=1,3
      T1=REFV(K,3)
      REFV(K,3)=REFV(K,2)
      REFV(K,2)=REFV(K,1)
  542 REFV(K,1)=T1
  552 CONTINUE
      IF(NJ2-3)670,582,599
  582 CALL MM(AA,WRKV,AAWRK)
      GO TO 699
  599 IF(NJ2-5)699,600,607
  600 IF(LATM-1)605,610,610
  605 NG=12
  606 CALL ERPNT(0.,506)
      CALL EXIT
  607 IF(NJ2-6)699,608,710
  608 IF(LATM-3)605,610,610
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  610 DO 612 J=1,3                                                      F500 920
      V2(J)=0.0                                                         F500 930
      DO 612 I=1,3                                                      F500 940
  612 RM(I,J)=0.0                                                       F500 950
      AWT=0.0                                                           F500 960
      DO 620 K=1,LATM                                                   F500 970
      CALL ATOM(ATOMS(1,K),ATOMS(2,K))                                  F500 980
      T2=1.0                                                            F500 990
      IF(NCD)618,618,613                                                F5001000
  613 I1=ATOMS(1,K)/100000.                                             F5001010
      DO 616 J=1,NCD                                                    F5001020
      T2=CD(1,J)                                                        F5001030
      IF(I1-KD(1,J))616,614,614                                         F5001040
  614 IF(KD(2,J)-I1)616,618,618                                         F5001050
  616 CONTINUE                                                          F5001060
      GO TO 620                                                         F5001070
  618 AWT=AWT+T2                                                        F5001080
      DO 619 J=1,3                                                      F5001090
  619 V2(J)=V2(J)+ATOMS(J+1,K)*T2                                       F5001100
  620 CONTINUE                                                          F5001110
      IF(AWT)605,605,621                                                F5001120
C     ***** PUT ORIGIN AT CENTER OF GRAVITY *****                       F5001130
  621 DO 622 J=1,3                                                      F5001140
  622 ORGN(J)=V2(J)/AWT                                                 F5001150
      IF(NJ2-6)699,624,710                                              F5001160
C     ***** FORM PRODUCT-MOMENT MATRIX FOR ATOMS IN ATOM LIST *****     F5001170
  624 DO 630 K=1,LATM                                                   F5001180
      T2=1.0                                                            F5001190
      IF(NCD)628,628,625                                                F5001200
  625 I1=ATOMS(1,K)/100000.                                             F5001210
      DO 627 J=1,NCD                                                    F5001220
      T2=CD(1,J)                                                        F5001230
      IF(I1-KD(1,J))627,626,626                                         F5001240
  626 IF(KD(2,J)-I1)627,628,628                                         F5001250
  627 CONTINUE                                                          F5001260
      GO TO 630                                                         F5001270
  628 DO 629 J=1,3                                                      F5001280
      T1=(ATOMS(J+1,K)-ORGN(J))*T2                                      F5001290
      DO 629 I=1,3                                                      F5001300
  629 RM(I,J)=T1*(ATOMS(I+1,K)-ORGN(I))+RM(I,J)                         F5001310
      T1=0.03/(RM(1,1)+RM(2,2)+RM(3,3))                                 F5001320
  630 CONTINUE                                                          F5001330
      DO 632 J=1,3                                                      F5001340
      DO 632 I=1,3                                                      F5001350
  632 RM(I,J)=RM(I,J)*T1                                                F5001360
C     ***** TRANSFORM TO INERTIAL AXIS SYSTEM *****                     F5001370
      CALL MM(RM,AA,DA)                                                 F5001380
      CALL EIGEN(DA,RMS,PAT)                                            F5001390
      IF(RMS(2))605,605,635                                             F5001400
  635 IF(NG)640,633,606                                                 F5001410
C     ***** MAKE SURE VECTORS ARE ORTHOGONAL --> NEW REFERENCE VECTORS *F5001420
  633 CALL AXES(PAT(1,3),PAT(1,1),REFV,-1)                              F5001430
      GO TO 665                                                         F5001440
C     ***** TWO EQUAL EIGENVECTORS SPECIAL CASE *****                   F5001450
  640 IF(NG+6)665,665,645                                               F5001460
  645 N=NG+5                                                            F5001470
      CALL UNIT(PAT(1,N),V1,-1)                                         F5001480
      DO 650 K=1,3                                                      F5001490
      IF(ABS(VMV(V1,AA,REFV(1,K)))-.58)655,650,650                      F5001500
  650 CONTINUE                                                          F5001510
  655 CALL AXES(V1,REFV(1,K),DA,-1)                                     F5001520
      DO 660 K=1,3                                                      F5001530
      L=MOD(N-K+2,3)+1                                                  F5001540
      DO 660 J=1,3                                                      F5001550
  660 REFV(J,L)=DA(J,K)                                                 F5001560
  665 NG=0                                                              F5001570
  670 CALL MM(AA,REFV,AAREV)                                            F5001580
  675 DO 680 J=1,3                                                      F5001590
      DO 680 I=1,3                                                      F5001600
      WRKV(I,J)=REFV(I,J)                                               F5001610
  680 AAWRK(I,J)=AAREV(I,J)                                             F5001620
C     ***** ELIMINATE ALL PREVIOUSLY STORED OVERLAP INFORMATION ****    F5001630
C     ***** (ALL INSTRUCTIONS FROM 501 THROUGH 510 DO THIS *****        F5001640
  699 CALL LAP500(0)                                                    F5001650
      GO TO 710                                                         F5001660
C     ***** STORE NEW OVERLAP INFORMATION (INSTRUCTION 511) *****       F5001670
  700 CALL LAP500(1)                                                    F5001680
  710 RETURN                                                            F5001690
      END                                                               F5001700
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      SUBROUTINE F600                                                   F600  10
C     ***** SCALING AND CENTERING FUNCTIONS *****                       F600  20
      DIMENSION MAX(3),SCAL(4),X(3),XMAX(3),XMIN(3),Z(2)                F600  30
      REAL*8 CHEM                                                       F600  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F600  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)F600  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F600  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F600  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F600  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F600 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F600 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F600 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD F600 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F600 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F600 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F600 160
C     ***** DEL = 1. FOR INCRUMENTING FUNCTIONS *****                   F600 170
C     ***** DEL = 0. FOR REGULAR FUNCTIONS *****                        F600 180
      DEI=FLOAT(MOD(NJ2/10,2))                                          F600 190
      NJ2=MOD(NJ2,10)                                                   F600 200
C     ***** EXPLICIT ORIGIN AND SCALE *****                             F600 210
      IF(AIN(1))602,604,602                                             F600 220
  602 XO(1)=AIN(1)+XO(1)*DEL                                            F600 230
  604 IF(AIN(2))606,608,606                                             F600 240
  606 XO(2)=AIN(2)+XO(2)*DEL                                            F600 250
  608 IF(AIN(3))612,612,609                                             F600 260
  609 IF(DEL)611,611,610                                                F600 270
  610 SCAL1=SCAL1*AIN(3)                                                F600 280
      GO TO 612                                                         F600 290
  611 SCAL1=AIN(3)                                                      F600 300
  612 IF(AIN(4))616,616,614                                             F600 310
C     ***** SET ELLIPSOID SCALE FACTOR *****                            F600 320
  614 SCAL2=AIN(4)                                                      F600 330
C     ***** AUTOMATIC ORIGIN AND/OR SCALE *****                         F600 340
  616 IF(NJ2-2)790,622,620                                              F600 350
  620 XO(1)=XLNG(1)*.5                                                  F600 360
      XO(2)=XLNG(2)*.5                                                  F600 370
  622 IF(NJ2-3)625,640,625                                              F600 380
  625 SCAL1=1.                                                          F600 390
  630 IF(LATM-1)635,635,640                                             F600 400
  635 NG=12                                                             F600 410
      CALL ERPNT(0.,602)                                                F600 420
      CALL EXIT                                                         F600 430
  640 DO 650 J=1,3                                                      F600 440
      XMAX(J)=-1.E5                                                     F600 450
  650 XMIN(J)=1.E5                                                      F600 460
C     ***** FIT BOX AROUND SET OF ATOMS *****                           F600 470
      DO 670 I=1,LATM                                                   F600 480
      CALL XYZ(ATOMS(1,I),ATOMS(2,I),3)                                 F600 490
      IF(NG)652,653,652                                                 F600 500
  652 CALL ERPNT(ATOMS(1,I),600)                                        F600 510
      GO TO 670                                                         F600 520
  653 DO 668 J=1,3                                                      F600 530
      T1=ATOMS(J+1,I)                                                   F600 540
      IF(XMAX(J)-T1)655,660,660                                         F600 550
  655 XMAX(J)=T1                                                        F600 560
      MAX(J)=I                                                          F600 570
  660 IF(T1-XMIN(J))665,668,668                                         F600 580
  665 XMIN(J)=T1                                                        F600 590
  668 CONTINUE                                                          F600 600
  670 CONTINUE                                                          F600 610
C     ***** KM=TOP ATOM *****                                           F600 620
      KM=MAX(3)                                                         F600 630
      SMULT=1.                                                          F600 640
      DO 780 M=1,5                                                      F600 650
      IF(M-2)740,675,678                                                F600 660
C     ***** CHECK VIEW DISTANCE *****                                   F600 670
  675 IF(VIEW)785,785,680                                               F600 680
  678 IF(NJ2-3)680,785,680                                              F600 690
  680 T1=ATOMS(4,KM)*SMULT                                              F600 700
      IF(VIEW*.5-T1)685,690,690                                         F600 710
C     ***** INCREASE VIEW DISTANCE *****                                F600 720
  685 VIEW=2.*T1                                                        F600 730
C     ***** FIND PERSPECTIVE PROJECTION LIMITS *****                    F600 740
  690 DO 700 J=1,2                                                      F600 750
      XMAX(J)=-1.E5                                                     F600 760
  700 XMIN(J)=1.E5                                                      F600 770
      DO 725 I=1,LATM                                                   F600 780
      DO 705 J=1,3                                                      F600 790
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  705 X(J)=ATOMS(J+1,I)*SMULT                                          F600 800
      T2=VIEW/(VIEW-X(3))                                              F600 810
      DO 725 J=1,2                                                     F600 820
      T1=X(J)*T2                                                       F600 830
      IF(XMAX(J)-T1)710,715,715                                        F600 840
  710 XMAX(J)=T1                                                       F600 850
  715 IF(T1-XMIN(J))720,725,725                                        F600 860
  720 XMIN(J)=T1                                                       F600 870
  725 CONTINUE                                                         F600 880
C     ***** REFINE PARAMETERS *****                                    F600 890
  740 IF(NJ2 -3)745,742,755                                            F600 900
  742 SMUL2=1.                                                         F600 910
      GO TO 765                                                        F600 920
C     ***** AUTOMATIC SCALE ONLY *****                                 F600 930
  745 DO 750 J=1,2                                                     F600 940
      T2=XO(J)                                                         F600 950
      SCAL(J)=(BRDR-T2)/XMIN(J)                                        F600 960
  750 SCAL(J+2)=(XLNG(J)-BRDR-T2)/XMAX(J)                              F600 970
      SMUL2=AMIN1(SCAL(1),SCAL(2),SCAL(3),SCAL(4))                     F600 980
      GO TO 780                                                        F600 990
C     ***** AUTOMATIC SCALE AND POSITION *****                         F6001000
  755 DO 760 J=1,2                                                     F6001010
  760 SCAL(J)=(XLNG(J)-BRDR*2.)/(XMAX(J)-XMIN(J))                      F6001020
      SMUL2=AMIN1(SCAL(1),SCAL(2))                                     F6001030
C     ***** AUTOMATIC POSITION *****                                   F6001040
  765 DO 770 J=1,2                                                     F6001050
  770 XO(J)=.5*(XLNG(J)-SMUL2*(XMAX(J)+XMIN(J)))                       F6001060
  780 SMULT=SMULT*SMUL2                                                F6001070
      VIEW=VIEW*SMUL2                                                  F6001080
  785 SCAL1=SCAL1*SMULT                                                F6001090
  790 SCL=SCAL1*SCAL2                                                  F6001100
C     ***** ELIMINATE ALL PREVIOUSLY STORED OVERLAP INFORMATION *****  F6001110
      CALL LAP500(0)                                                   F6001120
      RETURN                                                           F6001130
      END                                                              F6001140


      SUBROUTINE F700                                                  F700  10
C     ***** SUBROUTINE TO DRAW ELLIPSOIDS *****                        F700  20
      DIMENSION EYE(3),VIEWV(3),X(3),Z(3)                              F700  30
      REAL*8 CHEM                                                      F700  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)   F700  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F700  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F700  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F700  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)  F700  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)  F700 100
      DIMENSION XLNG(3),XO(3),XT(3)                                    F700 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D  F700 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F700 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F700 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2  F700 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                               F700 160
C     ***** SET ELLIPSOID GRAPHIC DETAILS *****                        F700 170
      ITILT=0                                                          F700 180
      NG=0                                                             F700 190
      NFIRST=1                                                         F700 200
      NPLANE=AIN(1)                                                    F700 210
      IF(NPLANE-1)720,715,720                                          F700 220
  715 NFIRST=4                                                         F700 230
      NPLANE=4                                                         F700 240
  720 NSOLID=AIN(2)                                                    F700 250
      NDOT=64/2**( IABS(NSOLID))                                       F700 260
      LINES=AIN(3)                                                     F700 270
      NDASH=AIN(4)                                                     F700 280
      CHSYM=AIN(5)                                                     F700 290
      DH=AIN(6)-CHSYM*17./7.                                           F700 300
      DV=AIN(7)-CHSYM*.5                                               F700 310
C     ***** ESTABLISH REFERENCE POINT OF VIEW *****                    F700 320
      T1=1.E6                                                          F700 330
      IF(VIEW) 740,740,735                                             F700 340
  735 T1=VIEW/SCAL1                                                    F700 350
  740 DO 741 J=1,3                                                     F700 360
  741 EYE(J)=REFV(J,3)*T1+ORGN(J)                                      F700 370
       LNS=-1                                                          F700 380
C     ***** LOOP THROUGH ATOM LIST *****                               F700 390
      DO 1105 ITOM=1,LATM                                              F700 400
      T1=ATOMS(1,ITOM)                                                 F700 410
      IF(AIN(10))744,744,742                                           F700 420
  742 T2=AINT(T1/100000.)                                              F700 430
      IF(T2-AIN(10))1105,743,743                                       F700 440
  743 IF(AIN(11)-T2)1105,744,744                                       F700 450
  744 CALL XYZ(T1,X,2)                                                 F700 460
      IF(NG) 758,746,758                                               F700 470
  746 CALL PLTXY(X,Z)                                                  F700 480
      K=T1/100000.                                                     F700 490
      L=T1-FLOAT (K)*100000.                                           F700 500
      IF(NJ2-10) 747,754,754                                           F700 510
  747 LNS=MOD(LNS+1,18)                                                F700 520
      IF(LNS) 749,748,749                                              F700 530
  748 WRITE (NOUT,751) (TITLE(I),I=1,18)                               F700 540
      WRITE (NOUT,752)                                                 F700 550
  749 WRITE (NOUT,750)CHEM(K),K,L,Z(1),Z(2),(X(I),I=1,3),(XT(          F700 560
     1I),I=1,3)                                                        F700 570
  750 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)    2F8.2,3X,3F8.3,11X,3F8.4)  F700 580
  751 FORMAT(1H110X,18A4)                                              F700 590
  752 FORMAT(1H010X,18HSYMBOL   ATOM CODE7X,16HPLOTTER X,Y(IN.) 3X,21HCAF700 600
     1RTESIAN X,Y,Z (IN.)15X,20HCRYSTAL SYSTEM X,Y,Z/1H 19X,45H(DIRECTIOF700 610
     2N COSINES(I,J),I=1,3),RMSD(J)),J=1,312X,42HFOR PRINCIPAL AXES BASEF700 620
     3D ON WORKING SYSTEM/1H )                                         F700 630
  754 IF(EDGE-BRDR*.75)755,760,760                                     F700 640
  755 NG=10                                                            F700 650
  758 CALL ERPNT(T1,700)                                               F700 660
      GO TO 1105                                                       F700 670
C     ***** CALL OVERLAP ROUTINE *****                                 F700 680
  760 ICQ=0                                                            F700 690
      CALL LAP700(ITOM,ICQ)                                            F700 700
      IF(ICQ) 762,764,764                                              F700 710
C     ***** OMIT HIDDEN ATOM *****                                     F700 720
  762 NG=14                                                            F700 730
      GO TO 758                                                        F700 740
  764 IF(CHSYM) 775,775,765                                            F700 750
C     ***** PLOT CHEMICAL SYMBOLS *****                                F700 760
  765 T4=1.                                                            F700 770
      IF(VIEW) 767,767,766                                             F700 780
  766 T4=VIEW/(VIEW-X(3))                                              F700 790
  767 T3=CHSYM*T4                                                      F700 800
      T4=DISP*T4*.5                                                    F700 810
      V1(1)=X(1)+DH*SYMB(1,1)+DV*SYMB(1,2)                             F700 820
      V1(2)=X(2)+DH*SYMB(2,1)+DV*SYMB(2,2)                             F700 830
      V1(3)=X(3)                                                       F700 840
      CALL PLTXY(V1,V3)                                                F700 850
      IF(EDGE-CHSYM) 775,768,768                                       F700 860
  768 V2(3)=0.                                                         F700 870
      DO 770 I=1,3,2                                                   F700 880
      V2(1)=V3(1)+FLOAT(I-2)*T4                                        F700 890
      DO 770 J=1,3,2                                                   F700 900
      V2(2)=V3(2)+FLOAT(J-2)*T4                                        F700 910
      CALL SIMBOL(V2(1),V2(2),T3,CHEM(K),THETA,6)                      F700 920
      IF(T4) 775,775,770                                               F700 930
  770 CONTINUE                                                         F700 940
  775 IF(NPLANE) 1105,1105,780                                         F700 950
C     ***** ELLIPSOID PRINC VECTORS TOWARD VIEWER *****                F700 960
  780 CALL PAXES(T1,2)                                                 F700 970
      IF(NG) 758,783,758                                               F700 980
  783 CALL DIFV(EYE,XT,VIEWV)                                          F700 990
      CALL UNIT(VIEWV,VIEWV,-1)                                        F7001000
      CALL VM(VIEWV,AA,V2)                                             F7001010
      DO 795 I=1,3                                                     F7001020
      IF(VV(V2,PAT(1,I)))785,795,795                                   F7001030
  785 DO 790 J=1,3                                                     F7001040
      PAC(J,I)=-PAC(J,I)                                               F7001050
  790 PAT(J,I)=-PAT(J,I)                                               F7001060
  795 CONTINUE                                                         F7001070
      DO 800 J=1,3                                                     F7001080
      PAC(J,4)=PAC(J,1)                                                F7001090
  800 PAC(J,5)=PAC(J,2)                                                F7001100
      IF(NJ2-10) 802,803,803                                           F7001110
  801 FORMAT(1H 13X,3(3X,3F8.4,F8.5)/1H )                              F7001120
  802 WRITE (NOUT,801) ((PAC(J,K),J=1,3),RMS(K) ,K=1,3)                F7001130
C     ***** V4 = VECTOR NORMAL TO POLAR PLANE *****                    F7001140
  803 CALL VM(VIEWV,AAWRK,V6)                                          F7001150
      CALL UNIT(V6,V6,1)                                               F7001160
      CALL MV(Q,V6,V4)                                                 F7001170
      CALL UNIT(V4,V4,1)                                               F7001180
C     ***** SET PLOTTING RESOLUTION FOR ELLIPSOID *****                F7001190
      T3=RMS(3)*SCL                                                    F7001200
      NRESOL=1                                                         F7001210
      NBIS=5                                                           F7001220
      DO 805 J=1,3                                                     F7001230
      IF(T3-RES(J))804,810,810                                         F7001240
  804 NBIS=NBIS-1                                                      F7001250
  805 NRESOL=NRESOL*2                                                  F7001260
  810 NRES1=NRESOL+1                                                   F7001270
C     ***** LOOP THROUGH PRINC AND POLAR PLANES *****                  F7001280
      DO 1100 II=NFIRST,NPLANE                                         F7001290
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      II0=MOD(II+2,3)+1                                                 F7001300
      II1=MOD(II,3)+1                                                   F7001310
      II2=MOD(II+1,3)+1                                                 F7001320
C     ***** GENERATE CONJUGATE DIAMETERS *****                          F7001330
      IF(.99938- ABS(VV(V4,PAC(1,II2))))820,820,830                     F7001340
  820 T1=RMS(II0)*SCL                                                   F7001350
      T2=RMS(II1)*SCL                                                   F7001360
      DO 825 J=1,3                                                      F7001370
      DA(J,1)=PAC(J,II0)*T1                                             F7001380
  825 DA(J,2)=PAC(J,II1)*T2                                             F7001390
      GO TO 850                                                         F7001400
  830 CALL NORM(PAC(1,II0),PAC(1,II1),V1,1)                             F7001410
      CALL NORM(V1,V4,V2,1)                                             F7001420
      CALL UNIT(V2,V2,1)                                                F7001430
      CALL MV(Q,V2,V3)                                                  F7001440
      IF(II-4) 835,840,840                                              F7001450
  835 CALL NORM(V3,V1,V5,1)                                             F7001460
      GO TO 843                                                         F7001470
  840 CALL NORM(V3,V4,V5,1)                                             F7001480
  843 CALL UNIT(V5,V5,1)                                                F7001490
      T1=SCL/SQRT(VMV(V2,Q,V2))                                         F7001500
      T2=SCL/SQRT(VMV(V5,Q,V5))                                         F7001510
      DO 845 J=1,3                                                      F7001520
      DA(J,1)=V2(J)*T1                                                  F7001530
  845 DA(J,2)=V5(J)*T2                                                  F7001540
C     ***** GENERATE ELLIPSE *****                                      F7001550
  850 CALL RADIAL(NBIS)                                                 F7001560
      IF(II-4) 900,851,851                                              F7001570
  851 IF(NSOLID) 859,859,852                                            F7001580
C     ***** PLOT DOTTED BOUNDARY ELLIPSE *****                          F7001590
  852 IF(NDOT-NRESOL) 853,855,855                                       F7001600
  853 CALL RADIAL(NSOLID-1)                                             F7001610
  855 CALL PROJ(D,DP,X,XO,VIEW,1,129,NDOT)                              F7001620
      DO 857 J=1,129,NDOT                                               F7001630
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    F7001640
      DO 856 I=1,3,2                                                    F7001650
      T1=FLOAT(I-2)*DISP                                                F7001660
      DO 856 K=1,3,2                                                    F7001670
      T2=FLOAT(K-2)*DISP                                                F7001680
      CALL DRAW(DP(1,J),T1,T2,2)                                        F7001690
      IF(DISP) 857,857,856                                              F7001700
  856 CONTINUE                                                          F7001710
  857 CONTINUE                                                          F7001720
      GO TO 1100                                                        F7001730
C     ***** PLOT SOLID BOUNDARY ELLIPSE *****                           F7001740
  859 CALL PROJ(D,DP,X,XO,VIEW,1,129,NRESOL)                            F7001750
      CALL DRAW(DP,0.,0.,3)                                             F7001760
      DO 860 J=NRES1,129,NRESOL                                         F7001770
  860 CALL DRAW(DP(1,J),0.,0.,2)                                        F7001780
      IF(DISP) 1100,1100,865                                            F7001790
C     ***** BOUNDARY ANNULUS AS A LINEAR FUNCTION OF HEIGHT *****       F7001800
  865 CALL DIFV(XT,ORGN,V1)                                             F7001810
      T5=VV(V1,AAREV(1,3))*SCAL1                                        F7001820
      NCYCLE=.5+(AIN(8)+T5*AIN(9))/DISP                                 F7001830
      IF(NCYCLE) 1100,1100,870                                          F7001840
  870 T3=(2.*DISP)/(T1+T2)                                              F7001850
C     ***** INCREASE ANNULAR THICKNESS *****                            F7001860
      DO 875 I=1,NCYCLE                                                 F7001870
      T4=T3*FLOAT(I)                                                    F7001880
      DO 875 J=1,129,NRESOL                                             F7001890
  875 CALL DRAW(DP(1,J),D(1,J)*T4,D(2,J)*T4,2)                          F7001900
      GO TO 1100                                                        F7001910
  900 CALL PROJ(D,DP,X,XO,VIEW,1,65,NRESOL)                             F7001920
C     ***** PLOT HALF AN ELLIPSE *****                                  F7001930
      CALL DRAW(DP,0.,0.,3)                                             F7001940
      DO 905 J=NRES1,65,NRESOL                                          F7001950
  905 CALL DRAW(DP(1,J),0.,0.,2)                                        F7001960
      IF(DISP) 930,930,910                                              F7001970
C     ***** ACCENTUATE FRONT HALF *****                                 F7001980
  910 DO 925 I=1,3,2                                                    F7001990
      T2=FLOAT(I-2)*DISP                                                F7002000
      DO 915 J=1,65,NRESOL                                              F7002010
      K=66-J                                                            F7002020
  915 CALL DRAW(DP(1,K),DISP,T2,2)                                      F7002030
      DO 925 K=1,65,NRESOL                                              F7002040
  925 CALL DRAW(DP(1,K),-DISP,-T2,2)                                    F7002050
  930 IF(NSOLID) 940,967,935                                            F7002060
  935 L=NDOT                                                            F7002070
      IF(NDOT-NRESOL) 938,945,940                                       F7002080
  938 CALL RADIAL(NSOLID-1)                                             F7002090
      GO TO 945                                                         F7002100
  940 L=NRESOL                                                          F7002110
  945 CALL PROJ(D(1,65),DP(1,65),X,XO,VIEW,1,65,L)                      F7002120
      IF(NSOLID) 960,967,950                                            F7002130
C     ***** DOTTED LINE ON REVERSE SIDE *****                           F7002140
  950 DO 958 J=65,129,NDOT                                              F7002150
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    F7002160
      DO 955 I=1,3,2                                                    F7002170
      T1=FLOAT(I-2)*DISP                                                F7002180
      DO 955 K=1,3,2                                                    F7002190
      T2=FLOAT(K-2)*DISP                                                F7002200
      CALL DRAW(DP(1,J),T1,T2,2)                                        F7002210
      IF(DISP) 958,958,955                                              F7002220
  955 CONTINUE                                                          F7002230
  958 CONTINUE                                                          F7002240
      GO TO 967                                                         F7002250
C     ***** SINGLE LINE ON REVERSE SIDE *****                           F7002260
  960 DO 965 J=65,129,NRESOL                                            F7002270
  965 CALL DRAW(DP(1,J),0.,0.,2)                                        F7002280
C     ***** DETAIL INTERIOR FEATURES *****                              F7002290
  967 T2=NDASH*2                                                        F7002300
      DO 975 J=1,3                                                      F7002310
      T1=PAC(J,II0)*RMS(II0)*SCL                                        F7002320
      DA(J,1)=T1                                                        F7002330
      DA(J,2)=PAC(J,II1)*RMS(II1)*SCL                                   F7002340
      DA(J,3)=0.                                                        F7002350
      IF(NDASH) 975,975,970                                             F7002360
  970 V1(J)=-T1                                                         F7002370
      V2(J)=T1/T2                                                       F7002380
  975 CONTINUE                                                          F7002390
      IF(NDASH) 987,987,980                                             F7002400
C     ***** DASHED LINE FOR REVERSE AXIS *****                          F7002410
  980 DO 985 J=1,NDASH                                                  F7002420
      DO 985 K=1,2                                                      F7002430
      L=4-K                                                             F7002440
      CALL PROJ(V1,DP,X,XO,VIEW,1,1,1)                                  F7002450
      CALL DRAW(DP,0.,0.,L)                                             F7002460
      DO 985 I=1,3                                                      F7002470
  985 V1(I)=V1(I)+V2(I)                                                 F7002480
C     ***** SOLID LINE FOR FORWARD AXIS *****                           F7002490
  987 IF(LINES) 1100,1100,988                                           F7002500
  988 CALL PROJ(DA,DP,X,XO,VIEW,1,3,1)                                  F7002510
      T1=DISP*.5                                                        F7002520
      DO 990 I=1,3,2                                                    F7002530
      T2=FLOAT(2-I)*T1                                                  F7002540
      CALL DRAW(DP,T1,T2,3)                                             F7002550
      CALL DRAW(DP(1,3),T1,T2,2)                                        F7002560
      IF(DISP) 1000,1000,989                                            F7002570
  989 CALL DRAW(DP(1,3),-T1,T2,2)                                       F7002580
  990 CALL DRAW(DP,-T1,T2,2)                                            F7002590
C     ***** SHADE QUADRANT BETWEEN TWO PRINCIPAL AXES *****             F7002600
 1000 L=LINES-1                                                         F7002610
      IF(L) 1100,1100,1005                                              F7002620
 1005 T2=LINES                                                          F7002630
      DO 1025 I=1,L                                                     F7002640
      T1=FLOAT(I)/T2                                                    F7002650
      T3=SQRT(1.-T1*T1)                                                 F7002660
      IF(MOD(I,2)) 1010,1015,1010                                       F7002670
 1010 M=I*2                                                             F7002680
      N=M-1                                                             F7002690
      GO TO 1020                                                        F7002700
 1015 N=I*2                                                             F7002710
      M=N-1                                                             F7002720
 1020 DO 1025 J=1,3                                                     F7002730
      T4=DA(J,1)*T1                                                     F7002740
      D(J,M)=T4                                                         F7002750
 1025 D(J,N)=DA(J,2)*T3+T4                                              F7002760
      L=L*2                                                             F7002770
      CALL PROJ(D,DP,X,XO,VIEW,1,L,1)                                   F7002780
      DO 1030 I=2,L,2                                                   F7002790
      CALL DRAW(DP(1,I-1),0.,0.,3)                                      F7002800
 1030 CALL DRAW(DP(1,I),0.,0.,2)                                        F7002810
 1100 CONTINUE                                                          F7002820
 1105 CONTINUE                                                          F7002830
C     ***** ELIMINATE LOCAL OVERLAP INFORMATION BEFORE RETURNING *****  F7002840
      CALL LAP500(-1)                                                   F7002850
      RETURN                                                            F7002860
      END                                                               F7002870


      SUBROUTINE F800                                                   F800  10
C     ***** SUBROUTINE FINDS ATOM PAIRS FOR BONDS *****                 F800  20
      DIMENSION IA(3),W1(6)                                             F800  30
      REAL*8 CHEM                                                       F800  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F800  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F800  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F800  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAI(3,3),Q(3,3),REFV(3,3) F800  80
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      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F800  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F800 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     F800 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F800 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F800 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F800 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F800 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F800 160
      LNS=-4                                                            F800 170
      IF(MOD(NJ2,10)-2) 805,848,848                                     F800 180
C     ***** EXPLICIT DESCRIPTION *****                                  F800 190
  805 II=0                                                              F800 200
      IF(NCD) 810,810,815                                               F800 210
  810 NG=11                                                             F800 220
      CALL ERPNT(0.,NJ*100+NJ2)                                         F800 230
      GO TO 980                                                         F800 240
  815 II=II+1                                                           F800 250
      IF(140-II) 980,980,820                                            F800 260
  820 T1=AIN(II)                                                        F800 270
      IF(T1) 815,815,825                                                F800 280
  825 II=II+1                                                           F800 290
      T2=AIN(II)                                                        F800 300
      IF(T2) 815,815,830                                                F800 310
  830 IF(NJ2-10) 832,838,838                                            F800 320
  832 LNS=MOD(LNS+4,56)                                                 F800 330
      IF(LNS) 838,834,838                                               F800 340
  834 WRITE (NOUT,835) (TITLE(I),I=1,18)                                F800 350
  835 FORMAT(1H110X,18A4)                                               F800 360
      WRITE (NOUT,837)                                                  F800 370
  837 FORMAT(1H010X,18HSYMBOL   ATCM CODE6X,16HPLOTTER X,Y(IN.) 6X,21HCAF800 380
     1RTESIAN X,Y,Z (IN.) 17X,20HCRYSTAL SYSTEM X,Y,Z/1H )              F800 390
C     ***** CHECK IF BOND ATOMS ARE IN ATOMS LIST (FOR OVERLAP CALC) ***F800 400
  838 NA1=0                                                             F800 410
      NA2=0                                                             F800 420
      IF(LATM-2) 845,839,839                                            F800 430
  839 N2=2                                                              F800 440
      DO 844 K=1,LATM                                                   F800 450
      T3=ATOMS(1,K)                                                     F800 460
      IF(T3-T1) 841,840,841                                             F800 470
  840 NA1=K                                                             F800 480
      GO TO 843                                                         F800 490
  841 IF(T3-T2) 844,842,844                                             F800 500
  842 NA2=K                                                             F800 510
  843 N2=N2-1                                                           F800 520
      IF(N2) 845,845,844                                                F800 530
  844 CONTINUE                                                          F800 540
  845 IF(NA2-NA1) 846,847,847                                           F800 550
  846 NA3=NA1                                                           F800 560
      NA1=NA2                                                           F800 570
      NA2=NA3                                                           F800 580
      T3=T1                                                             F800 590
      T1=T2                                                             F800 600
      T2=T3                                                             F800 610
  847 CALL BOND(T1,T2,1,NA1,NA2)                                        F800 620
      GO TO 815                                                         F800 630
C     ***** IMPLICIT DESCRIPTION *****                                  F800 640
  848 IF(LATM-2) 810,850,850                                            F800 650
  850 SCAL3=SCAL1                                                       F800 660
      SCAL1=1.                                                          F800 670
      DO 855 I=1,LATM                                                   F800 680
  855 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                 F800 690
      SCAL1=SCAL3                                                       F800 700
      IF(NCD) 810,810,860                                               F800 710
  860 WRITE (NOUT,861)                                                  F800 720
  861 FORMAT(1H010X,20HBOND SELECTION CODES//11X,94H(SEQUENCE(A)) (SEQUENF800 730
     1CE(B)) (BOND) (DISTANCES) ( BOND ) (PERSP.--LABELS) (NORMAL--LABELS) (F800 740
     2DIGITS) /11X,93H(  MIN   MAX )(  MIN   MAX ) (TYPE) (MIN    MAX) (RADIF800 750
     3US) (HEIGHT  OFFSET) (HEIGHT  OFFSET) (NUMBER))                   F800 760
      DMAX=0.                                                           F800 770
      DO 870 I=1,NCD                                                    F800 780
      IF(DMAX-CD(2,I)) 865,870,870                                      F800 790
  865 DMAX=CD(2,I)                                                      F800 800
  870 WRITE (NOUT,871) (KD(J,I),J=1,5),(CD(J,I),J=1,8)                  F800 810
  871 FORMAT(1H 10XI6,I5,I8,I5,I8,2F6.2,5F8.3,F7.0)                     F800 820
      DMAX=DMAX*DMAX                                                    F800 830
C     ***** LOOP THROUGH ATOMS ARRAY *****                              F800 840
      DO 977 M=1,LATM                                                   F800 850
      NA1=M                                                             F800 860
      T1=ATOMS(1,M)                                                     F800 870
      IA(1)=T1/100000.                                                  F800 880
      IA(3)=IA(1)                                                       F800 890
      W1(1)=ATOMS(2,M)                                                  F800 900
      W1(2)=ATOMS(3,M)                                                  F800 910
      W1(3)=ATOMS(4,M)                                                  F800 920
      L=M+1                                                             F800 930
      IF(LATM-L) 977,872,872                                            F800 940
  872 DO 975 N=L,LATM                                                   F800 950
      NA2=N                                                             F800 960
      DIST=(ATOMS(2,N)-W1(1))**2                                        F800 970
      IF(DMAX-DIST) 975,873,873                                         F800 980
  873 DIST=DIST+(ATOMS(3,N)-W1(2))**2                                   F800 990
      IF(DMAX-DIST) 975,874,874                                         F8001000
  874 DIST=DIST+(ATOMS(4,N)-W1(3))**2                                   F8001010
      IF(DMAX-DIST) 975,875,875                                         F8001020
  875 DIST=SQRT(DIST)                                                   F8001030
      T2=ATOMS(1,N)                                                     F8001040
      IA(2)=T2/100000.                                                  F8001050
C     ***** SELECT BONDS ACCORDING TO CODES *****                       F8001060
      DO 950 J=1,NCD                                                    F8001070
      JB=J                                                              F8001080
      IF(DIST-CD(1,J))    950,880,880                                   F8001090
  880 IF(CD(2,J)-DIST)    950,881,881                                   F8001100
  881 DO 885 K=1,2                                                      F8001110
      IF(IA(K)-KD(1,J))   885,882,882                                   F8001120
  882 IF(KD(2,J)-IA(K))   885,883,883                                   F8001130
  883 IF(IA(K+1)-KD(3,J)) 885,884,884                                   F8001140
  884 IF(KD(4,J)-IA(K+1)) 885,890,890                                   F8001150
  885 CONTINUE                                                          F8001160
      GO TO 950                                                         F8001170
C     ***** CHECK FOR POLYHEDRA CODE *****                              F8001180
  890 IF(CD(4,J)) 900,955,955                                           F8001190
  900 W1(4)=ATOMS(2,N)                                                  F8001200
      W1(5)=ATOMS(3,N)                                                  F8001210
      W1(6)=ATOMS(4,N)                                                  F8001220
      KM1=ABS(CD(4,J))                                                  F8001230
      KM2=ABS(CD(5,J))                                                  F8001240
      DSQ1=(CD(6,J))**2                                                 F8001250
      DSQ2=(CD(7,J))**2                                                 F8001260
C     ***** SEARCH FOR POLYHEDRA CENTER *****                           F8001270
      DO 935 IM=1,LATM                                                  F8001280
      K3=ATOMS(1,IM)/100000.                                            F8001290
      IF(K3-KM1) 935,905,905                                            F8001300
  905 IF(KM2-K3) 935,910,910                                            F8001310
C     ***** CHECK POLYHEDRA DISTANCE RANGE *****                        F8001320
  910 DO 930 J1=1,4,3                                                   F8001330
      DSQ=(ATOMS(2,IM)-W1(J1))**2                                       F8001340
      IF(DSQ2-DSQ) 935,915,915                                          F8001350
  915 DSQ=DSQ+(ATOMS(3,IM)-W1(J1+1))**2                                 F8001360
      IF(DSQ2-DSQ) 935,920,920                                          F8001370
  920 DSQ=DSQ+(ATOMS(4,IM)-W1(J1+2))**2                                 F8001380
      IF(DSQ2-DSQ) 935,925,925                                          F8001390
  925 IF(DSQ-DSQ1) 935,930,930                                          F8001400
  930 CONTINUE                                                          F8001410
      GO TO 955                                                         F8001420
  935 CONTINUE                                                          F8001430
C     ***** END OF POLYHEDRA CHECK *****                                F8001440
  950 CONTINUE                                                          F8001450
      GO TO 975                                                         F8001460
C     ***** PREPARE TO DRAW BOND *****                                  F8001470
  955 IF(NJ2-10) 960,970,970                                            F8001480
  960 LNS=MOD(LNS+4,56)                                                 F8001490
      IF(LNS) 965,965,970                                               F8001500
  965 WRITE (NOUT,835) (TITLE(I),I=1,18)                                F8001510
      WRITE (NOUT,837)                                                  F8001520
  970 CALL BOND(T1,T2,JB,NA1,NA2)                                       F8001530
  975 CONTINUE                                                          F8001540
  977 CONTINUE                                                          F8001550
C     ***** ELIMINATE LOCAL OVERLAP INFORMATION BEFORE RETURNING *****  F8001560
  980 IF(NJ2-21) 985,990,990                                            F8001570
  985 CALL LAP500(-1)                                                   F8001580
  990 RETURN                                                            F8001590
      END                                                               F8001600


      SUBROUTINE F900                                                   F900  10
      DIMENSION X(3),XW(3,5),Y(3),Z(3)                                  F900  20
      REAL*8 CHEM                                                       F900  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F900  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)F900  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F900  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F900  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F900  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F900  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     F900 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F900 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F900 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F900 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F900 140
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      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F900 150
C     ***** LABELING FUNCTION SUBROUTINE *****                          F900 160
      ITILT=0                                                           F900 170
      NJ3=MOD(NJ2,10)                                                   F900 180
      TH=THETA                                                          F900 190
      SINTH=SYMB(2,1)                                                   F900 200
      COSTH=SYMB(1,1)                                                   F900 210
      ILAST=1                                                           F900 220
      IF(AIN(2)-11100.)910,910,905                                      F900 230
  905 ILAST=2                                                           F900 240
  910 DO 925 II=1,ILAST                                                 F900 250
C     ***** OBTAIN WORKING CARTESIAN COORDINATES *****                  F900 260
      CALL XYZ(AIN(II),XW(1,II),2)                                      F900 270
      IF(NG)915,925,915                                                 F900 280
  912 NG=15                                                             F900 290
  915 CALL ERPNT(AIN(II),NJ*100+NJ2)                                    F900 300
      GO TO 1199                                                        F900 310
  925 CALL XYZ(AIN(II),XW(1,II+3),3)                                    F900 320
      II=1                                                              F900 330
C     ***** FIND MEAN REFERENCE POINT *****                             F900 340
      DO 930 J=1,3                                                      F900 350
      T2=XW(J,ILAST)                                                    F900 360
      T1=XW(J,1)                                                        F900 370
      XW(J,3)=T2-T1                                                     F900 380
  930 X(J)=(T2+T1)*.5                                                   F900 390
C     ***** PERSPECTIVE SCALING FACTOR *****                            F900 400
      SCAL=1.                                                           F900 410
      IF(VIEW)940,940,935                                               F900 420
  935 SCAL=VIEW/(VIEW-X(3))                                             F900 430
  940 HGT=SCAL*AIN(5)                                                   F900 440
      IF(NJ2-3)960,950,945                                              F900 450
  945 IF(NJ2-6)950,950,960                                              F900 460
C     ***** PROJECTED VECTOR BASELINE *****                             F900 470
  950 CALL PLTXY(XW(1,4),V1)                                            F900 480
      CALL PLTXY(XW(1,5),V2)                                            F900 490
      T1=V2(1)-V1(1)                                                    F900 500
      T2=V2(2)-V1(2)                                                    F900 510
      T3=SQRT(T1*T1+T2*T2)                                              F900 520
      IF(T3)912,912,955                                                 F900 530
  955 COSTH=T1/T3                                                       F900 540
      SINTH=T2/T3                                                       F900 550
      TH=ARCCOS(COSTH)                                                  F900 560
      IF(SINTH)958,960,960                                              F900 570
  958 TH=-TH                                                            F900 580
  960 IF(NJ2-13)965,985,985                                             F900 590
C     ***** FIND CENTER OF PROJECTED LABEL *****                        F900 600
  965 Y(1)=SCAL*(X(1)+AIN(6)*COSTH-AIN(7)*SINTH)+XO(1)                  F900 610
      Y(2)=SCAL*(X(2)+AIN(6)*SINTH+AIN(7)*COSTH)+XO(2)                  F900 620
      Y(3)=0.                                                           F900 630
C     ***** CHECK FOR LEGEND RESET *****                                F900 640
      DO 980 J=1,2                                                      F900 650
      T1=AIN(J+2)                                                       F900 660
      IF(T1)975,980,970                                                 F900 670
  970 Y(J)=T1                                                           F900 680
      GO TO 980                                                         F900 690
  975 Y(J)=XLNG(J)+T1                                                   F900 700
  980 CONTINUE                                                          F900 710
C     ***** SET PARAMETERS FOR INDIVIDUAL FUNCTIONS *****               F900 720
  985 GO TO(990,995,995,1000,1000,1000,915,1105,1105,915,915,915,1005,10F900 730
     105,1005,1005,915),NJ2                                             F900 740
  990 T6=17.                                                            F900 750
      L=AIN(1)/100000.                                                  F900 760
      ILAST=1                                                           F900 770
      DXW=0.                                                            F900 780
      DYW=0.                                                            F900 790
      GO TO 1030                                                        F900 800
  995 T6=215.                                                           F900 810
      ILAST=18                                                          F900 820
      T1=HGT*24./7.                                                     F900 830
      DXW=COSTH*T1                                                      F900 840
      DYW=SINTH*T1                                                      F900 850
      GO TO 1030                                                        F900 860
 1000 T6=10+3*(NJ3-4)                                                   F900 870
      DIST=SQRT(VV(XW(1,3),XW(1,3)))/SCAL1                              F900 880
      GO TO 1030                                                        F900 890
C     ***** TRUE PERSPECTIVE LABELS *****                               F900 900
 1005 CALL UNIT(XW(1,3),VT(1,1),1)                                      F900 910
      IF(ABS(VT(3,1))-.9994)1010,912,912                                F900 920
C     ***** FORM PERSPECTIVE ROTATION MATRIX *****                      F900 930
 1010 CALL NORM(AID(1,3),VT(1,1),VT(1,2),1)                             F900 940
      CALL UNIT(VT(1,2),VT(1,2),1)                                      F900 950
      CALL NORM(VT(1,1),VT(1,2),VT(1,3),1)                              F900 960
      DO 1015 J=1,3                                                     F900 970
 1015 VT(J,4)=X(J)                                                      F900 980
      ITILT=1                                                           F900 990
      HGT=AIN(5)                                                        F9001000
      TH=0.                                                             F9001010
      Y(3)=X(3)                                                         F9001020
      Y(2)=X(2)+AIN(7)-HGT*.5                                           F9001030
      IF(NJ2-13)1030,1025,1020                                          F9001040
C     ***** PERSPECTIVE BOND LABELS *****                               F9001050
 1020 Y(1)=X(1)+AIN(6)-HGT*FLOAT(22+3*(6-NJ3))/7.                       F9001060
      DIST=SQRT(VV(XW(1,3),XW(1,3)))/SCAL1                              F9001070
      GO TO 1050                                                        F9001080
C     ***** PERSPECTIVE TITLES *****                                    F9001090
 1025 Y(1)=X(1)+AIN(6)-HGT*215./7.                                      F9001100
      ILAST=18                                                          F9001110
      DXW=HGT*24./7.                                                    F9001120
      DYW=0.                                                            F9001130
      GO TO 1050                                                        F9001140
 1030 DH=HGT*T6/7.                                                      F9001150
      DV=HGT*.5                                                         F9001160
      Y(1)=Y(1)-DH*COSTH+DV*SINTH                                       F9001170
      Y(2)=Y(2)-DH*SINTH-DV*COSTH                                       F9001180
      Y(3)=0.                                                           F9001190
C     ***** PLOT VARIOUS LABELS *****                                   F9001200
 1050 Z(3)=Y(3)                                                         F9001210
      XO(3)=Y(3)                                                        F9001220
      GO TO(1060,1060,1060,1090,1090,1090,915,1105,1105),NJ3            F9001230
 1060 DO 1085 I=1,ILAST                                                 F9001240
      DO 1075 J=1,3,2                                                   F9001250
      Z(1)=Y(1)+FLOAT(J-2)*DISP*.5                                      F9001260
      DO 1075 K=1,3,2                                                   F9001270
      Z(2)=Y(2)+FLOAT(K-2)*DISP*.5                                      F9001280
      IF(NJ3-2)1065,1068,1068                                           F9001290
C     ***** PLOT CHEMICAL SYMBOL *****                                  F9001300
 1065 CALL SIMBOL(Z(1),Z(2),HGT,CHEM(L),TH,6)                           F9001310
      GO TO 1070                                                        F9001320
C     ***** PLOT TITLES *****                                           F9001330
 1068 CALL SIMBOL(Z(1),Z(2),HGT,TITLE2(I),TH,4)                         F9001340
 1070 IF(DISP)1080,1080,1075                                            F9001350
 1075 CONTINUE                                                          F9001360
 1080 Y(1)=Y(1)+DXW                                                     F9001370
 1085 Y(2)=Y(2)+DYW                                                     F9001380
      GO TO 1199                                                        F9001390
C     ***** PLOT BOND DISTANCE LABELS *****                             F9001400
 1090 I9=NJ3-3                                                          F9001410
      T9=10.**I9                                                        F9001420
      DISTR=AINT((DIST*T9)+0.5)/T9 +.0001                               F9001430
      CALL NUMBUF(Y(1),Y(2),HGT,DISTR,TH,I9)                            F9001440
      GO TO 1199                                                        F9001450
C     ***** PLOT CENTERED SYMBOLS *****                                 F9001460
 1105 CALL SIMBOL(Y(1),Y(2),HGT, IFIX(AIN(8)),TH,7-NJ3)                 F9001470
 1199 ITILT=0                                                           F9001480
      RETURN                                                            F9001490
      END                                                               F9001500


      SUBROUTINE F1000                                                  F100  10
      DIMENSION D6(3,3),D15(15),D6L(3,3),DQ(6),QQ(6)                    F100  20
      DIMENSION C1(3),QF(3,3),C3(10),CE(10)                             F100  30
      DIMENSION CIJK(3,3,3),GAMMA(3,3,3),B2(3,3),B3(3,3)                F100  40
      DIMENSION Z0(3),Z1(3),Z2(3),DZ0(3),DZ1(3),LINE(22,2),HEAD(22)     F100  50
      REAL*8 CHEM                                                       F100  60
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F100  70
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) F100  80
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) F100  90
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F100 100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   F100 110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F100 120
      DIMENSION XLNG(3),XO(3),XT(3)                                     F100 130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F100 140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD F100 150
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F100 160
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F100 170
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F100 180
      EQUIVALENCE(LINE(1),HEAD(1))                                      F100 190
C**** SUBROUTINE TO ANALYZE TENSORS OF HIGHER CUMULANTS ****            F100 200
C     COLUMN  6- 9  = 1000                                              F100 210
C     COLUMN 10-18 FIRST ATOM WITH SKEW TENSOR, IF 0 OR BLANK IS SET = 1F100 220
C     COLUMN 19-27 LAST ATOM WITH SKEW TENSOR, IF ZERO IS SET = NATOM   F100 230
C     COLUMN 28-36 IF ZERO SHIFT POSITION PARAMETERS OF ATOM TO MODE    F100 240
C                  IF .GT. ZERO, DO NOT SHIFT TO MODE                   F100 250
C     COLUMN 37-45 PSI AND CHI IF ZERO, ONLY PSI IF +, ONLY CHI IF MINUSF100 260
C**** CONTINUATION CARD IF A 1 IN COLUMN 3 OF PREVIOUS CARD ****        F100 270
C     COLUMN 10-18 SCALE FACTOR FOR MAPS, IF ZERO, NO MAPS              F100 280
C     COLUMN 19-27 NUMBER OF GRID POINTS ALONG X IN MAP                 F100 290
C     COLUMN 28-36                                 Y                    F100 300
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C      COLUMN 37-45                                  Z
C      COLUMN 46-54 INCREMENT ALONG X IN ANGSTROMS
C      COLUMN 55-63                    Y
C      COLUMN 64-67                    Z
C**** CONTINUATION CARD IF A 1 IN COLUMN 3 OF PREVIOUS CARD ****
C      COLUMN 10-18 MID-POINT IN RANGE OF X
C      COLUMN 19-27                             Y
C      COLUMN 28-36                             Z
C      COLUMN 37-45 NON-ZERO TO READ AND SUBTRACT RIGID-BODY CUMULANTS
C      COLUMN 46-54 SCALE FACTOR FOR REGULAR    CUMULANTS IN SUBTRACTION
C      COLUMN 55-63 SCALE FACTOR FOR RIGID BODY CUMULANTS IN SUBTRACTION
C      COLUMN 64-72 NON-ZERO TO READ OLD FORMAT 3K(I,J,K) CARDS
       NA1 = AIN(1)
       IF(NA1)200,200,205
   200 NA1 = 1
   205 NA2 = AIN(2)
       IF(NA2)210,210,215
   210 NA2 = NATOM
   215 DO 505 IA = NA1,NA2
C      ***** READ IN FIRST AND SECOND CUMULANT TENSORS *****
       READ(IN,2) CHEM2,SCAT,FRAC,(V6(J),J=1,3),B2(1,1),B2(2,2),B2(3,3)
      1,B2(1,2),B2(1,3),B2(2,3),ALPHA,IBE,IGM,IDL
     2 FORMAT (A6,3X,5F9.5,26X / 6F9.6,F7.4,2X,3I3)
       CONST=0.001
       IF(AIN(21))2152,2152,2151
  2151 CONST=1./41.34170
       GO TO 220
  2152 IF(IGM-1)222,217,216
   216 IF(IGM-3)220,217,220
C      ***** READ CONTRACTED GAMMA TENSOR (COVARIANT FORM) *****
   217 READ (IN,4)(C1(J),J=1,3)
     4 FORMAT (5E14.7,10X)
       IGM=3
       GO TO 222
C      ***** READ FULL GAMMA TENSOR (CONTRAVARIANT FORM) *****
   220 READ (IN,4)CIJK(1,1,1),CIJK(2,2,2),CIJK(3,3,3),CIJK(1,1,2)
      1,CIJK(1,2,2),CIJK(1,1,3),CIJK(1,3,3),CIJK(2,2,3),CIJK(2,3,3)
      2,CIJK(1,2,3)
       IGM=10
   222 IF(IDL-1)241,225,223
   223 IF(IDL-3)226,227,224
   224 IF(IDL-15)226,227,241
C      ***** READ DELTA TENSOR *****
   225 READ (IN,4) D1
       IDL=1
       GO TO 241
   226 READ (IN,4) D6(1,1),D6(2,2),D6(3,3),D6(1,2),D6(1,3),D6(2,3)
       IDL=6
       GO TO 241
   227 READ (IN,4) D15(1),D15(11),D15(15),D15(2),D15(7),D15(3),D15(10)
      1,D15(12),D15(14),D15(4),D15(6),D15(13),D15(5),D15(8),D15(9)
       IDL=15
C      ***** EXPAND BETA2 TENSOR,MULTIPLY BY 2 / (4 * PI**2) *****
   241 DO 242 I=1,3
       DO 242 J=I,3
       B2(I,J)=B2(I,J)*5.06605918E-2
   242 B2(J,I)=B2(I,J)
       IF(IGM-3)2501,243,247
   243 IF(ALPHA)500,500,244
C      ***** EXPAND CONTRACTED GAMMA TENSOR *****
   244 T1=0.2E5/ALPHA**2
       DO 245 J=1,3
   245 V2(J)=C1(J)*T1
       CALL MV(B2,V2,C1)
       DO 246 I=1,3
       DO 246 J=I,3
       DO 246 K=J,3
   246 CIJK(I,J,K)= C1(I)*B2(J,K)+C1(K)*B2(I,J)+C1(J)*B2(K,I)
   247 IF(AIN(18))235,249,235
C      ***** READ AND SUBTRACT OUT RIGID-BODY CONTRIBUTION *****
   235 READ(IN,2)CHEM3,SCAT3,FRAC,(V5(J),J=1,3),B3(1,1),B3(2,2),B3(3,3)
      1,B3(1,2),B3(1,3),B3(2,3)
       READ (IN,4)
      1GAMMA(1,1,1),GAMMA(2,2,2),GAMMA(3,3,3),GAMMA(1,1,2),GAMMA(1,2,2)
      2,GAMMA(1,1,3),GAMMA(1,3,3),GAMMA(2,2,3),GAMMA(2,3,3),GAMMA(1,2,3)
       DO 240 I = 1,3
       DO 240 J = I,3
       DO 240 K = J,3
   240 CIJK(I,J,K) = CIJK(I,J,K)*AIN(19)-GAMMA(I,J,K)*AIN(20)
   249 DO 250 I=1,3
       DO 250 J=I,3
       DO 250 K = J,3
       T1 = CIJK(I,J,K)*CONST
       CIJK(I,J,K) = T1
       CIJK(K,I,J) = T1
       CIJK(J,K,I) = T1
       CIJK(K,J,I) = T1
       CIJK(I,K,J) = T1
   250 CIJK(J,I,K) = T1
C      ***** EXPAND CONTRACTED DELTA TENSORS *****
  2501 IF(IDL-1)260,251,253
   251 D1=D1*128.0
       DO 252 I=1,3
       DO 252 J=1,3
   252 D6(I,J)=B2(I,J)*D1/3.0
   253 IF(IDL-6)256,254,260
C      ***** CONVERT TO CONTRAVARIANT FORM *****
   254 T1=28./(.01*ALPHA**3)
       DO 255 I=1,3
       DO 255 J=I,3
       D6L(I,J)=D6(I,J)*T1
   255 D6L(J,I)=D6L(I,J)
       CALL MM(B2,D6L,DA)
       CALL MM(DA,B2,D6)
C      ***** EXPAND TO 4TH ORDER TENSOR *****
   256 IJKL=0
       DO 257 I=1,3
       DO 257 J=I,3
       DO 257 K=J,3
       DO 257 L=K,3
       IJKL=IJKL+1
   257 D15(IJKL)=(B2(I,J)*D6(K,L)+B2(I,K)*D6(J,L)+B2(I,L)*D6(J,K)
      1          +B2(K,L)*D6(I,J)+B2(J,L)*D6(I,K)+B2(J,K)*D6(I,L))/7.0
C      ***** INVERT BETA MATRIX *****
   260 CALL PAXES(FLOAT(IA)*100000.+55501.,1)
C      ***** STORE IN ARRAY WITH PROPER MULTIPLICITY *****
       IJ=0
       DO 262 I=1,3
       DO 262 J=I,3
       IJ=IJ+1
       T1=2.0
       IF(I-J)262,261,262
   261 T1=1.0
   262 QQ(IJ)=Q(I,J)*T1
       IF(IDL-6)270,267,263
C      ***** CONTRACT 4TH ORDER DELTA TENSOR *****
   263 IJ=0
       DO 265 I=1,3
       DO 265 J=1,I
       IJ=IJ+1
       DQ(IJ)=0.0
       N=IJ-I
       KL=0
       DO 265 K=1,3
       N=N+I-1
       DO 265 L=1,K
       KL=KL+1
       N=N+1
   265 DQ(IJ)=DQ(IJ) + QQ(KL)*D15(N)
       IJ=0
       DO 266 I=1,3
       DO 266 J=I,3
       IJ=IJ+1
       D6(I,J)=DQ(IJ)
   266 D6(J,I)=DQ(IJ)
C      ***** CONTRACT 2NT ORDER DELTA TENSOR
   267 D1=0.0
       DO 268 I=1,3
       DO 268 J=1,3
   268 D1=D1+Q(I,J)*D6(I,J)
   270 IF(IGM-3)500,275,275
C      ***** CONTRACT GAMMA TENSOR *****
   275 DO 285 K = 1,3
       T1 = 0.0
       DO 280 J = 1,3
       VT(K,J) = PA(K,J,IA)/EV(J,IA)
       DO 280 I = 1,3
   280 T1 = T1 + CIJK(I,J,K)* Q(I,J)
   285 V1(K) = T1
       DO 290 J = 1,3
C      ***** FORM FIRST CUMULANT - MEAN DIFFERENCE VECTOR IN V5 *****
       V5(J) = V6(J) - P(J,IA) + 0.5 * ALPHA * V1(J)
       V4(J) = EV(J,IA)**2
   290 V3(J) = 1.0 / V4(J)
       WRITE(NOUT,8) (TITLE(I),I=1,18)
     8 FORMAT(1H1,10X,18A4)
       WRITE (NOUT,10)
    10 FORMAT(1H0, 9H NO. ATOM,5X,5H1L(1),6X,5H1L(2),6X,5H1L(3),  3X,33H(
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     1CONTRACTED 3K(I,I,J) =  3K(J)) =,3X,5H3K(1),6X,5H3K(2),6X,5H3K(3)/F1001950
     21H ,14X,7H3K(111),4X,7H3K(222),4X,7H3K(333),4X,7H3K(112),4X,      F1001960
     37H3K(122),4X,7H3K(113),4X,7H3K(133),4X,7H3K(223),4X,7H3K(233),3X, F1001970
     47H3K(123))                                                        F1001980
      WRITE (NOUT,12)                                                   F1001990
   12 FORMAT(1H0,22HCRYSTAL OBLIQUE SYSTEM)                             F1002000
      WRITE (NOUT,14) IA,CHEM(IA),(V5(J),J=1,3),(V1(J),J=1,3),          F1002010
     1CIJK(1,1,1),CIJK(2,2,2),CIJK(3,3,3),CIJK(1,1,2),CIJK(1,2,2),      F1002020
     2CIJK(1,1,3),CIJK(1,3,3),CIJK(2,2,3),CIJK(2,3,3),CIJK(1,2,3)       F1002030
   14 FORMAT(1H ,I3,1X,A6,3F11.8,33X,3F11.8/1H ,10X,9F11.8,F10.8)       F1002040
      WRITE (NOUT,16)                                                   F1002050
   16 FORMAT(1H0,26HREFERENCE CARTESIAN SYSTEM)                         F1002060
C     ***** TRANSFORMATION MATRIX FOR REFERENCE CARTESIAN SYSTEM *****  F1002070
      DO 295 J = 1,9                                                    F1002080
  295 PAC(J,1) = AAREV(J,1)                                             F1002090
      ISYS = 0                                                          F1002100
      GO TO 305                                                         F1002110
C     ***** REPLACE REFERENCE SYSTEM BY PRINCIPAL AXIS SYSTEM *****     F1002120
  300 CALL MM(AA,VT,PAC)                                                F1002130
      WRITE (NOUT,18)                                                   F1002140
   18 FORMAT(1H0,35HUNIT VARIANCE PRINCIPAL-AXIS SYSTEM)                F1002150
C     ***** TRANSFORM GAMMA TENSCR TO ORTHOGONAL SYSTEM *****          F1002160
  305 DO 315 N = 1,3                                                    F1002170
      DO 315 M = N,3                                                    F1002180
      DO 315 L = M,3                                                    F1002190
      T1 = 0.0                                                          F1002200
      DO 310 K = 1,3                                                    F1002210
      T2 = PAC(K,N)                                                     F1002220
      DO 310 J = 1,3                                                    F1002230
      T3 = T2 * PAC(J,M)                                                F1002240
      DO 310 I = 1,3                                                    F1002250
  310 T1 = T1 + CIJK(I,J,K)*PAC(I,L)*T3                                 F1002260
      GAMMA(L,M,N) = T1                                                 F1002270
      GAMMA(N,L,M) = T1                                                 F1002280
      GAMMA(M,N,L) = T1                                                 F1002290
      GAMMA(N,M,L) = T1                                                 F1002300
      GAMMA(L,N,M) = T1                                                 F1002310
  315 GAMMA(M,L,N) = T1                                                 F1002320
C     ***** TRANSFORM VECTORS TO ORTHOGONAL SYSTEM *****               F1002330
      DO 320 J = 1,3                                                    F1002340
      V2(J) = 0.0                                                       F1002350
      V4(J) = 0.0                                                       F1002360
      V6(J) = 0.0                                                       F1002370
      DO 320 I = 1,3                                                    F1002380
      V6(J) = V6(J) + V1(I)*PAC(I,J)                                    F1002390
  320 V4(J) = V4(J) + V5(I)*PAC(I,J)                                    F1002400
  325 WRITE (NOUT,20)IA,CHEM(IA),(V4(J),J=1,3),(V6(J),J=1,3)            F1002410
     1,GAMMA(1,1,1),GAMMA(2,2,2),GAMMA(3,3,3),GAMMA(1,1,2),GAMMA(1,2,2) F1002420
     2,GAMMA(1,1,3),GAMMA(1,3,3),GAMMA(2,2,3),GAMMA(2,3,3),GAMMA(1,2,3) F1002430
   20 FORMAT(1H ,I3,1X,A6,3F11.6,33X,3F11.6/1H ,10X,9F11.6,F10.6)       F1002440
      IF(ISYS) 330 ,330 ,340                                            F1002450
C     ***** STORE 1L(I),3K(I,J,K) AND INVERSE OF 2K(I,J) FOR EDGE SERIESF1002460
  330 CALL PAXES(FLOAT(IA)*100000.+55501.,3)                            F1002470
      IJK = 1                                                           F1002480
      DO 335  I = 1,3                                                   F1002490
      C1(I) = V4(I)                                                     F1002500
      DO 335  J = I,3                                                   F1002510
      QF(J,I) = Q(J,I)                                                  F1002520
      QF(I,J) = Q(I,J)                                                  F1002530
      DO 335  K = J,3                                                   F1002540
      C3(IJK) = GAMMA(I,J,K)*0.5                                        F1002550
  335 IJK = IJK + 1                                                     F1002560
      C3(1) = C3(1)/3.0                                                 F1002570
      C3(7) = C3(7)/3.0                                                 F1002580
      C3(10) = C3(10)/3.0                                               F1002590
      C3(5) = C3(5)*2.0                                                 F1002600
      CALL PAXES(FLOAT(IA)*100000.+55501.,-3)                           F1002610
      GO TO 350                                                         F1002620
  340 DO 345 I = 1,9                                                    F1002630
  345 Q(I,1) = AID(I,1)                                                 F1002640
C     ***** EXPAND THE CONTRACTED VECTOR *****                         F1002650
  350 IJK = 1                                                           F1002660
      DO 355 I = 1,3                                                    F1002670
      DO 355 J = I,3                                                    F1002680
      DO 355 K = J,3                                                    F1002690
      CE(IJK) = 0.2*(V6(I)*Q(J,K)+V6(J)*Q(K,I)+V6(K)*Q(I,J))            F1002700
  355 IJK = IJK + 1                                                     F1002710
      WRITE (NOUT,22) CE(1),CE(7),CE(10),CE(2),CE(4),CE(3),CE(6),CE(8)  F1002720
     1,CE(9),CE(5)                                                      F1002730
   22 FORMAT(11H XPND 3K(J),9F11.6,F10.6)                               F1002740
      ISYS = ISYS + 1                                                   F1002750
      IF(ISYS-1) 300,300,360                                            F1002760
C     ***** MULTIPLY TERMS IN BASIC UNIT OF GAMMA BY THEIR MULTIPLICITY F1002770
  360 GAMMA(1,1,2) = GAMMA(1,1,2)*3.0                                   F1002780
      GAMMA(1,2,2) = GAMMA(1,2,2)*3.0                                   F1002790
      GAMMA(1,1,3) = GAMMA(1,1,3)*3.0                                   F1002800
      GAMMA(1,3,3) = GAMMA(1,3,3)*3.0                                   F1002810
      GAMMA(2,2,3) = GAMMA(2,2,3)*3.0                                   F1002820
      GAMMA(2,3,3) = GAMMA(2,3,3)*3.0                                   F1002830
      GAMMA(1,2,3) = GAMMA(1,2,3)*6.0                                   F1002840
C     ***** CALCULATE MODE OF PROBABILITY DENSITY FUNCTION *****       F1002850
      T4 = 0.0                                                          F1002860
      DO 365 J = 1,3                                                    F1002870
      V2(J) = V4(J)-V6(J)*0.5                                           F1002880
  365 T4 = T4 + V2(J)**2                                                F1002890
      T4 = SQRT(T4)                                                     F1002900
      IF(T4-1.0) 380,380,370                                            F1002910
  370 DO 375 J = 1,3                                                    F1002920
  375 V2(J) = V2(J)/T4                                                  F1002930
  380 CALL HERMIT(V2,V4,GAMMA,PSI,CHI,EV(1,IA),1)                       F1002940
      T4 = 0.0                                                          F1002950
      DO 385 J = 1,3                                                    F1002960
      T1 = EV(J,IA)                                                     F1002970
      V2(J) = V2(J)*T1                                                  F1002980
  385 T4 = T4 + V2(J)**2                                                F1002990
      T4 = SQRT(T4)                                                     F1003000
C     ***** SHIFT POSITIONAL PARAMETERS TO MODE *****                  F1003010
      DO 395 J = 1,3                                                    F1003020
      V6(J) = P(J,IA)                                                   F1003030
      XT(J) = V6(J)                                                     F1003040
      DO 390 I = 1,3                                                    F1003050
  390 P(J,IA) = P(J,IA) + V2(I)*PA(J,I,IA)                              F1003060
  395 V3(J) = P(J,IA) - V6(J)                                           F1003070
      WRITE (NOUT,24)                                                   F1003080
   24 FORMAT(1H0,15X,6HX MEAN,5X,6HY MEAN,5X,6HZ MEAN,16X,6HX MODE,5X,  F1003090
     16HY MODE,5X,6HZ MODE,20X,12HDISPLACEMENT)                         F1003100
      WRITE (NOUT,12)                                                   F1003110
      WRITE (NOUT,26)IA,CHEM(IA),(V6(J),J=1,3),(V3(J)   ,J=1,3),T4      F1003120
   26 FORMAT(1H ,I3,1X,A6,3F11.6,11X,3F11.6,16X,F6.3,1X,9HANGSTROMS)    F1003130
      T1 = 55501. + FLOAT(IA)*100000.                                   F1003140
      CALL XYZ(T1,V2,-3)                                                F1003150
      CALL XYZ(T1,V3,3)                                                 F1003160
      DO 400 J = 1,3                                                    F1003170
  400 V3(J) = V3(J) - V2(J)                                             F1003180
      IF(AIN(3)) 415,415,405                                            F1003190
  405 DO 410 J = 1,3                                                    F1003200
  410 P(J,IA) = V6(J)                                                   F1003210
      WRITE (NOUT,28)                                                   F1003220
   28 FORMAT(1H ,   29HPOSITIONAL PARAMETERS AT MEAN)                   F1003230
      GO TO 420                                                         F1003240
  415 WRITE (NOUT,30)                                                   F1003250
   30 FORMAT(1H ,   29HPOSITIONAL PARAMETERS AT MODE)                   F1003260
C     ***** PRINT MEAN AND MODE BASED ON REFERENCE CARTESIAN SYSTEM ****F1003270
  420 WRITE (NOUT,16)                                                   F1003280
      WRITE (NOUT,26)IA,CHEM(IA),(V2(J),J=1,3),(V3(J),J=1,3),T4         F1003290
C     ***** PRINT PRINCIPAL AXES BASED ON REFERENCE CARTESIAN SYSTEM ***F1003300
      WRITE (NOUT,32)                                                   F1003310
   32 FORMAT(1H0,10X,16HRMS DISPLACEMENT, 8X,31HROW VECTORS, BASED ON REF1003320
     1FERENCE,15X,28HCOVARIANCE MATRIX (U TENSOR))                      F1003330
      CALL PAXES(T1,-3)                                                 F1003340
      WRITE (NOUT,34) (RMS(J),(PAC(I,J),I=1,3),(Q(I,J),I=1,3),J=1,3)    F1003350
   34 FORMAT(1H0,10X,F11.4,11X,3F11.6,11X,3F11.6)                       F1003360
      IF(AIN(8)) 425,505,425                                            F1003370
C     ***** CALCULATE EDGEWORTH DENSITY MAP *****                      F1003380
  425 SCAT = AMIN1(SCAT,1.0)                                            F1003390
      SCAL3=.063493636 *AIN(8)*SCAT/(EV(1,IA)*EV(2,IA)*EV(3,IA))        F1003400
      DO 430 J = 1,3                                                    F1003410
      DZ0(J) = AIN(J+11)                                                F1003420
  430 Z0(J) = AIN(J+14) - 0.5*(AIN(J+8)+1.0)*AIN(J+11)                  F1003430
      NX = AIN(9)                                                       F1003440
      NY = AIN(10)                                                      F1003450
      NZ = AIN(11)                                                      F1003460
C     ***** LOOP OVER Z OF REFERENCE SYSTEM *****                      F1003470
      DO 500 IZ = 1,NZ                                                  F1003480
      DZ1(3) = FLOAT(IZ)                                                F1003490
      Z1(3) = Z0(3) + DZ0(3)*DZ1(3)                                     F1003500
      WRITE (NOUT,36)Z1(3),CHEM(IA)                                     F1003510
   36 FORMAT (13H1 SECTION Z =,F6.3,3X,A6)                              F1003520
      DO 435 I = 1,NY                                                   F1003530
  435 HEAD(I) = Z0(2) + DZ0(2)*FLOAT(I)                                 F1003540
      WRITE (NOUT,38) (HEAD(I),I=1,NY)                                  F1003550
   38 FORMAT(9H Y(A.U.)=,22F5.2)                                        F1003560
C     ***** LOOP OVER X OF REFERENCE SYSTEM *****                      F1003570
      DO 500 IX = 1,NX                                                  F1003580
      DZ1(1) = FLOAT(IX)                                                F1003590
      Z1(1) = Z0(1) + DZ0(1)*DZ1(1)                                     F1003600
C     ***** LOOP OVER Y OF REFERENCE SYSTEM *****                      F1003610
      DO 480 IY = 1,NY                                                  F1003620
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      DZ1(2) = FLOAT(IY)
      Z1(2) = Z0(2) + DZ0(2)*DZ1(2)                                     F1003630
C     ***** EVALUATE EDGEWORTH SERIES AT POINT Z1(I) *****              F1003640
      DO 440 I = 1,3                                                    F1003650
      Z2(I) = 0.0                                                       F1003660
      DO 440 J = 1,3                                                    F1003670
  440 Z2(I) = Z2(I) + Z1(J)*QF(J,I)                                     F1003680
      LILJLK = 1                                                        F1003690
      PSI = 1.0                                                         F1003700
      QUAD = 0.0                                                        F1003710
      DO 445 LI = 1,3                                                   F1003720
      Z2LI = Z2(LI)                                                     F1003730
      PSI = PSI + Z2LI*C1(LI)                                           F1003740
      QUAD = QUAD + Z2LI*Z1(LI)                                         F1003750
      DO 445 LJ = LI,3                                                  F1003760
      Z2LJ = Z2(LJ)                                                     F1003770
      ZIZJQF = Z2LI*Z2LJ - QF(LI,LJ)                                    F1003780
      DO 445 LK = LJ,3                                                  F1003790
      PSI = PSI + C3(LILJLK) * (Z2(LK)*ZIZJQF - Z2LI*QF(LK,LJ)          F1003800
     1- Z2LJ*QF(LK,LI))                                                 F1003810
  445 LILJLK = LILJLK + 1                                               F1003820
      PDF = SCAL3*EXP(-.5*QUAD)                                         F1003830
      CHI = PDF*(PSI-1.0)                                               F1003840
      PSI = PDF* PSI                                                    F1003850
C     ***** ROUND AND STORE PSI *****                                   F1003860
      T1 = PSI                                                          F1003870
      LTEMP = T1 + SIGN(0.5,T1)                                         F1003880
      IF(LTEMP)460,450,460                                              F1003890
  450 IF(T1 )455,460,460                                                F1003900
  455 LTEMP = -0                                                        F1003910
  460 LINE(IY,1) = LTEMP                                                F1003920
C     ***** ROUND AND STORE CHI *****                                   F1003930
      T1 = CHI                                                          F1003940
      LTEMP = T1 + SIGN(0.5,T1)                                         F1003950
      IF(LTEMP)475,465,475                                              F1003960
  465 IF(T1 )470,475,475                                                F1003970
  470 LTEMP = -0                                                        F1003980
  475 LINE(IY,2) = LTEMP                                                F1003990
  480 CONTINUE                                                          F1004000
C     ***** PRINT PSI AND CHI IF AIN(4).EQ.0 , ONLY PSI IF +, CHI IF - *F1004010
      IF(AIN(4)) 495,485,490                                            F1004020
  485 WRITE (NOUT,40)                                                   F1004030
      WRITE (NOUT,44)Z1(1),(LINE(J,1),J=1,NY)                           F1004040
      WRITE (NOUT,46)Z1(1),(LINE(J,2),J=1,NY)                           F1004050
      GO TO 500                                                         F1004060
  490 WRITE (NOUT,42)                                                   F1004070
      WRITE (NOUT,44)Z1(1),(LINE(J,1),J=1,NY)                           F1004080
      GO TO 500                                                         F1004090
  495 WRITE (NOUT,42)                                                   F1004100
      WRITE (NOUT,46)Z1(1),(LINE(J,2),J=1,NY)                           F1004110
   40 FORMAT(1H )                                                       F1004120
   42 FORMAT(1H0)                                                       F1004130
   44 FORMAT(3H XP, F6.3,22I5)                                          F1004140
   46 FORMAT(3H XC, F6.3,22I5)                                          F1004150
  500 CONTINUE                                                          F1004160
  505 CONTINUE                                                          F1004170
      RETURN                                                            F1004180
      END                                                               F1004190
                                                                        F1004200

      SUBROUTINE HERMIT(X,U,GAMMA,PSI,CHI,RMS,ITYPE)
C     ***** SUBROUTINE TO REFINE MODE *****                             HERM  10
      DIMENSION A(3,3),X(3),Y(3),GAMMA(3,3,3),H(6,3)        ,KH(4),V1(3) HERM  20
      DIMENSION  JT(5,10),IT(5),VALU(3),VECT(3,3),RMS(3),U(3)           HERM  30
C     ***** ITYPE=0, PSI, CHI CALC/.GT.0 MAXIMUM PHI/.LT.0 MAXIMUM CHI  HERM  40
      ICYCLE = 0                                                        HERM  50
      IF(ITYPE)205,200,210                                              HERM  60
  200 ASSIGN 435 TO NBY1                                                HERM  70
      ASSIGN 300 TO NBY2                                                HERM  80
      ASSIGN 435 TO NBY3                                                HERM  90
      ILAST = 1                                                         HERM 100
      GO TO 220                                                         HERM 110
  205 ASSIGN 435 TO NBY3                                                HERM 120
      ASSIGN 290 TO NBY2                                                HERM 130
      GO TO 215                                                         HERM 140
  210 ASSIGN 330 TO NBY3                                                HERM 150
      ASSIGN 285 TO NBY2                                                HERM 160
  215 ASSIGN 260 TO NBY1                                                HERM 170
      ILAST = 4                                                         HERM 180
  220 ICYCLE = ICYCLE + 1                                               HERM 190
      ASSIGN 235 TO I5BY                                                HERM 200
      ASSIGN 245 TO I4BY                                                HERM 210
      ASSIGN 270 TO I3BY                                                HERM 220
      ASSIGN 315 TO I2BY                                                HERM 230
      ASSIGN 355 TO I1BY                                                HERM 240
      PSI = 1.0                                                         HERM 250
C     ***** GENERATE H0,H1,...,H5 FOR X(IX),IX=1,3 *****                HERM 260
      DO 230 IX = 1,3                                                   HERM 270
      H(1,IX) = 1.0                                                     HERM 280
      XH = X(IX)                                                        HERM 290
      H(2,IX) = XH                                                      HERM 300
      HI = 1.0                                                          HERM 310
      DO 225 IH = 2,5                                                   HERM 320
      H(IH+1,IX) = XH*H(IH,IX) - HI*H(IH-1,IX)                          HERM 330
  225 HI = HI + 1.0                                                     HERM 340
      Y(IX) = 0.0                                                       HERM 350
      KH(IX) = 1                                                        HERM 360
      DO 230 J = 1,3                                                    HERM 370
C     ***** REDEFINE HERMITE POLYNOMIALS WITHOUT (-1)**N FACTOR *****   HERM 380
      JX2 = J*2                                                         HERM 390
      H(JX2,IX) = -H(JX2,IX)                                            HERM 400
  230 A(J,IX) = 0.0                                                     HERM 410
      KH(4) = 1                                                         HERM 420
C     ***** FORM TENSORS OF HERMITE POLYNOMIALS *****                   HERM 430
      DO 455 I1 = 1,ILAST                                               HERM 440
      I1M1 = I1 - 1                                                     HERM 450
      IT(1) = I1M1                                                      HERM 460
      KH(I1) = KH(I1) + 1                                               HERM 470
      DO 450 I2 =I1,ILAST                                               HERM 480
      I2M1 = I2 - 1                                                     HERM 490
      IT(2) = I2M1                                                      HERM 500
      KH(I2) = KH(I2) + 1                                               HERM 510
      DO 445 I3 = I2,4                                                  HERM 520
      I3M1 = I3 - 1                                                     HERM 530
      IT(3) = I3M1                                                      HERM 540
      KH(I3) = KH(I3) + 1                                               HERM 550
      DO 440 I4 = I3,4                                                  HERM 560
      I4M1 = I4 - 1                                                     HERM 570
      IT(4) = I4M1                                                      HERM 580
      KH(I4) = KH(I4) + 1                                               HERM 590
      DO 435 I5 = I4,4                                                  HERM 600
      I5M1 = I5-1                                                       HERM 610
      IT(5) = I5M1                                                      HERM 620
      KH(I5) = KH(I5) + 1                                               HERM 630
C     *****SKIP ZERO ORDER TERM *****                                   HERM 640
      GO TO I5BY,(235,240)                                              HERM 650
  235 ASSIGN 240 TO I5BY                                                HERM 660
      GO TO 435                                                         HERM 670
  240 K1 = KH(2)                                                        HERM 680
      K2 = KH(3)                                                        HERM 690
      K3 = KH(4)                                                        HERM 700
      TERM = H(K1,1)*H(K2,2)*H(K3,3)                                    HERM 710
      GO TO I4BY,(245,265)                                              HERM 720
  245 IF(I4M1) 255,255,250                                              HERM 730
  250 ASSIGN 265 TO I4BY                                                HERM 740
      GO TO 265                                                         HERM 750
C     ***** USE H(I) *****                                              HERM 760
C     ***** SUM SECOND PART OF PSI *****                                HERM 770
  255 PSI = PSI - TERM * U(I5M1)                                        HERM 780
      GO TO NBY1,(260,435)                                              HERM 790
C     ***** SUM FIRST PART OF VECTOR OF FIRST DERIVITIVES *****         HERM 800
  260 Y(I5M1) = Y(I5M1) - TERM                                          HERM 810
      GO TO 435                                                         HERM 820
  265 GO TO I3BY,(270,305)                                              HERM 830
  270 IF(I3M1) 280,280,275                                              HERM 840
  275 ASSIGN 305 TO I3BY                                                HERM 850
      GO TO 305                                                         HERM 860
C     ***** USE H(I)H(J) *****                                          HERM 870
  280 GO TO NBY2,(285,290,300)                                          HERM 880
C     ***** SUM FIRST PART OF MATRIX OF SECOND DERIVITIVES *****        HERM 890
  285 A(I4M1,I5M1) = A(I4M1,I5M1) + TERM                                HERM 900
C     ***** SUM SECOND PART OF VECTOR OF FIRST DERIVITIVES *****        HERM 910
  290 Y(I5M1) = Y(I5M1) + TERM * U(I4M1)                                HERM 920
      IF(I5M1-I4M1)435,435,295                                          HERM 930
  295 Y(I4M1) = Y(I4M1) + TERM * U(I5M1)                                HERM 940
      GO TO 435                                                         HERM 950
C     ***** SKIP H(I)H(J) PART IF CALCULATING PHI ONLY *****            HERM 960
  300 KH(I5) = KH(I5) - 1                                               HERM 970
      KH(I4) = KH(I4) - 1                                               HERM 980
      GO TO 445                                                         HERM 990
C     ***** CALCULATE CONSTANT*GAMMA(I,J,K)*HERMITE(I,J,K) *****        HERM1000
  305 TERM2 = GAMMA(I3M1,I4M1,I5M1)*TERM*0.16666667                     HERM1010
  310 GO TO I2BY,(315,350)                                              HERM1020
  315 IF(I2M1) 325,325,320                                              HERM1030
  320 ASSIGN 350 TO I2BY                                                HERM1040
      GO TO 350                                                         HERM1050
                                                                        HERM1060
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C     ***** USE H(I)H(J)H(K)  *****                                      HERM1070
C     ***** SUM THIRD PART OF PSI *****                                  HERM1080
  325 PSI = PSI - TERM2                                                   HERM1090
      GO TO NBY3,(330,435)                                                HERM1100
C     ***** SUM SECOND PART OF MATRIX OF SECOND DERIVITIVES *****        HERM1110
  330 A(I4M1,I5M1) = A(I4M1,I5M1) - TERM * U(I3M1)                        HERM1120
      IF(I5M1-I4M1)340,340,335                                            HERM1130
  335 A(I3M1,I4M1) = A(I3M1,I4M1) - TERM * U(I5M1)                        HERM1140
  340 IF(I4M1-I3M1)435,435,345                                            HERM1150
  345 A(I3M1,I5M1) = A(I3M1,I5M1) - TERM * U(I4M1)                        HERM1160
      GO TO 435                                                           HERM1170
  350 GO TO I1BY,(355,395)                                                HERM1180
  355 IF(I1M1) 365,365,360                                                HERM1190
  360 ASSIGN 395 TO I1BY                                                  HERM1200
      GO TO 395                                                           HERM1210
C     ***** USE H(I)H(J)H(K)H(L)  *****                                  HERM1220
C     ***** SUM THIRD PART OF VECTOR OF FIRST DERIVITIVES *****          HERM1230
  365 Y(I2M1) = Y(I2M1) + TERM2                                           HERM1240
      IF(I5M1-I4M1)375,375,370                                            HERM1250
  370 Y(I5M1) = Y(I5M1) + GAMMA(I2M1,I3M1,I4M1)*TERM*0.16666667           HERM1260
  375 IF(I4M1-I3M1)385,385,380                                            HERM1270
  380 Y(I4M1) = Y(I4M1) + GAMMA(I2M1,I3M1,I5M1)*TERM*0.16666667           HERM1280
  385 IF(I3M1-I2M1)435,435,390                                            HERM1290
  390 Y(I3M1) = Y(I3M1) + GAMMA(I2M1,I4M1,I5M1)*TERM*0.16666667           HERM1300
      GO TO 435                                                           HERM1310
C     ***** USE H(I)H(J)H(K)H(L)H(M)  *****                              HERM1320
C     ***** SUM THIRD PART OF MATRIX OF SECOND DERIVITIVES *****         HERM1330
C     ***** SET UP ORDERED PERMUTATIONS OF I1,I2,I3,I4,I5 BY 2 S, 3 S **HERM1340
  395 LT = 0                                                              HERM1350
      LB = 11                                                             HERM1360
      DO 410 I=1,4                                                        HERM1370
      IP1 = I+1                                                           HERM1380
      DO 410 J=IP1,5                                                      HERM1390
      LT = LT+1                                                           HERM1400
      JT(1,LT) = IT(I)                                                    HERM1410
      JT(2,LT) = IT(J)                                                    HERM1420
      IF(J-4)400,400,410                                                  HERM1430
  400 JP1 = J+1                                                           HERM1440
      DO 405 K=JP1,5                                                      HERM1450
      LB = LB-1                                                           HERM1460
      JT(3,LB) = IT(I)                                                    HERM1470
      JT(4,LB) = IT(J)                                                    HERM1480
  405 JT(5,LB) = IT(K)                                                    HERM1490
  410 CONTINUE                                                            HERM1500
C     ***** FIND UNIQUE ORDERED PERMUTATIONS OF I1,I2,I3,I4,I5 BY 2,3 S HERM1510
      J1 = 0                                                              HERM1520
      J2 = 0                                                              HERM1530
      J5 = 0                                                              HERM1540
      DO 430 J=1,10                                                       HERM1550
      IF((J1-3)*(J5-1))415,435,415                                        HERM1560
  415 IF(J1-JT(1,J))425,420,425                                           HERM1570
  420 IF(J2-JT(2,J))425,430,425                                           HERM1580
  425 J1 = JT(1,J)                                                        HERM1590
      J2 = JT(2,J)                                                        HERM1600
      J3 = JT(3,J)                                                        HERM1610
      J4 = JT(4,J)                                                        HERM1620
      J5 = JT(5,J)                                                        HERM1630
      A(J1,J2) = A(J1,J2) - GAMMA(J3,J4,J5)*TERM*0.16666667               HERM1640
  430 CONTINUE                                                            HERM1650
  435 KH(I5) = KH(I5) - 1                                                 HERM1660
  440 KH(I4) = KH(I4) - 1                                                 HERM1670
  445 KH(I3) = KH(I3) - 1                                                 HERM1680
  450 KH(I2) = KH(I2) - 1                                                 HERM1690
  455 KH(I1) = KH(I1) - 1                                                 HERM1700
C     ***** FILL OUT MATRIX A AND MULTIPLY A,Y AND PSI BY NORMAL DENSITYHERM1710
      DEN = 0.063493636 * EXP(-.5*(X(1)**2+X(2)**2+X(3)**2))              HERM1720
      PSI = PSI * DEN                                                     HERM1730
      CHI = PSI - DEN                                                     HERM1740
      IF(ITYPE)460,500,460                                                HERM1750
C     ***** NEGATE DENSITY FOR POSITIVE MATRIX A ON MAXIMA SEARCH ***** HERM1760
  460 DEN = -DEN                                                          HERM1770
      DO 470 I = 1,3                                                      HERM1780
      DO 465 J = I,3                                                      HERM1790
      A(I,J) = A(I,J)*DEN                                                 HERM1800
  465 A(J,I) = A(I,J)                                                     HERM1810
  470 Y(I) = Y(I) * DEN                                                   HERM1820
C     ***** CHECK EIGENVALUES OF MATRIX A *****                          HERM1830
      CALL EIGEN(A,VALU,VECT)                                             HERM1840
      IF(VALU(1))495,495,475                                              HERM1850
C     *****CALCULATE SHIFT VECTOR *****                                   HERM1860
  475 CALL AXEQB(A,V1,Y,1)                                                HERM1870
C     ***** CALCULATE LENGTH OF SHIFT VECTOR *****                        HERM1880
      T1 = 0.0                                                            HERM1890
      DO 480 J = 1,3                                                      HERM1900
      T1 = T1 + (V1(J)*RMS(J))**2                                         HERM1910
  480 X(J) = X(J) + V1(J)                                                 HERM1920
      IF(T1-1.0E-10)500,485,485                                           HERM1930
C     ***** ERROR IF SHIFT IS .GE. 0.3 A *****                           HERM1940
  485 IF(T1-0.09)490,495,495                                              HERM1950
  490 IF(ICYCLE-20)220,495,495                                            HERM1960
  495 PRINT 2,ICYCLE,VALU                                                 HERM1970
    2 FORMAT(22H0MODE FAILURE ON CYCLE,I3,3E20.5)                         HERM1980
      PRINT 4,PSI,CHI,T1,V1,X,VALU,Y,A,H                                  HERM1990
    4 FORMAT(1H0/(1H ,6E19.8))                                            HERM2000
  500 RETURN                                                              HERM2010
      END                                                                 HERM2020


      SUBROUTINE LAP500(NTYPE)                                            LAP5  10
C     ***** STORE PROJECTED ATOM CONICS AND BOND QUADRANGLES *****       LAP5  20
      DIMENSION QC(3,3),QD(3,3),VD1(3),VD2(3)                             LAP5  30
C     ***** DOUBLE PRECISION FOR VERY SMALL ATOMS AND SHORT WORDLENGTH *LAP5  40
C     ***** IN GENERAL, DOUBLE PRECISION IS NOT REQUIRED *****           LAP5  50
      REAL*8 QC,QD,VD1,VD2,TD1,TD2,TD3                                    LAP5  60
C     ***** JUST REMOVE THE PRECEEDING REAL*8 CARD TO MAKE SINGLE PREC   LAP5  70
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER,  LAP5  80
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)          LAP5  90
      REAL*8 CHEM                                                         LAP5 100
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      LAP5 110
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) LAP5 120
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)  LAP5 130
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  LAP5 140
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)    LAP5 150
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    LAP5 160
      DIMENSION XLNG(3),XO(3),XT(3)                                       LAP5 170
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D    LAP5 180
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD  LAP5 190
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALILAP5 200
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    LAP5 210
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                  LAP5 220
C     ***** ELIMINATE ALL PREVIOUSLY STORED LOCAL OVERLAP INFORMATION **LAP5 230
      NCOVER=0                                                            LAP5 240
      NQOVER=0                                                            LAP5 250
      IF(NTYPE)420,195,195                                                LAP5 260
C     ***** ELIMINATE ALL PREVIOUSLY STORED GLOBAL OVERLAP INFORMATION *LAP5 270
  195 NCONIC=0                                                            LAP5 280
      NQUAD=0                                                             LAP5 290
      IF(NTYPE)420,420,200                                                LAP5 300
C     ***** CONSTANT FOR OVERLAP MARGIN (WHITE MARGIN AT OVERLAP) ***** LAP5 310
  200 IF(AIN(1))205,215,210                                               LAP5 320
C     ***** NEGATIVE NUMBER OR POSITIVE INTEGER GIVES OVMRGN=0.0 *****  LAP5 330
  205 OVMRGN=0.0                                                          LAP5 340
      GO TO 220                                                           LAP5 350
C     ***** SET OVERLAP MARGIN WIDTH DIRECTLY IN INCHES *****            LAP5 360
  210 OVMRGN=AIN(1)-AINT(AIN(1))                                          LAP5 370
      GO TO 220                                                           LAP5 380
C      ***** DEFAULT OPTION, OVERLAP MARGIN WIDTH AS A FUNCTION OF SCALILAP5 390
  215 OVMRGN=AMAX1(SQRT(SCAL1)*0.030,0.025)                               LAP5 400
  220 WRITE (NOUT,2) OVMRGN                                               LAP5 410
    2 FORMAT(1H0,10X,17HOVERLAP MARGIN IS, F6.3,5H INCH)                  LAP5 420
  225 IF(LATM)230,230,235                                                 LAP5 430
  230 NG=12                                                               LAP5 440
      CALL ERPNT(0.,510+NJ2)                                              LAP5 450
      GO TO 420                                                           LAP5 460
C     ***** SORT ATOMS LIST BY -VIEWDISTANCE OR BY Z PARAMETER           LAP5 470
  235 IF(VIEW)250,250,240                                                 LAP5 480
C     ***** CALCULATE VIEWDISTANCES**2 *(-1) IF VIEW.GT.ZERO *****      LAP5 490
  240 DO 245 I=1,LATM                                                     LAP5 500
      CALL XYZ(ATOMS(1,I),V3,2)                                           LAP5 510
      V3(3)=V3(3)-VIEW                                                    LAP5 520
  245 ATOMS(4,I)=-VV(V3,V3)                                               LAP5 530
      GO TO 260                                                           LAP5 540
C     ***** STORE CARTESIAN COORDINATES IF VIEW.EQ.ZERO *****            LAP5 550
  250 DO 255 I=1,LATM                                                     LAP5 560
  255 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                   LAP5 570
C     ***** SORTING PROCEDURE BY SHELL, COMM ACM 2,30 (1959) *****       LAP5 580
  260 M=LATM                                                              LAP5 590
  265 M=M/2                                                               LAP5 600
      IF(M)300,300,270                                                    LAP5 610
  270 K=LATM-M                                                            LAP5 620
      J=1                                                                 LAP5 630
  275 I=J                                                                 LAP5 640
  280 IM=I+M                                                              LAP5 650
      IF(ATOMS(4,I)-ATOMS(4,IM))295,295,285                               LAP5 660
  285 DO 290 L=1,4,3                                                      LAP5 670
      T1=ATOMS(L,I)                                                       LAP5 680
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      ATOMS(L,I)=ATOMS(L,IM)                                            LAP5 690
  290 ATOMS(L,IM)=T1                                                    LAP5 700
      I=I-M                                                             LAP5 710
      IF(I)295,295,280                                                  LAP5 720
  295 J=J+1                                                             LAP5 730
      IF(J-K)275,275,265                                                LAP5 740
C     ***** LOOP THROUGH ALL ATOMS IN SORTED ATOMS LIST *****           LAP5 750
  300 DO 405 IA=1,LATM                                                  LAP5 760
      CALL XYZ(ATOMS(1,IA),ATOMS(2,IA),2)                               LAP5 770
      CALL PAXES(ATOMS(1,IA),2)                                         LAP5 780
      DO 305 J=1,3                                                      LAP5 790
      V1(J)=ATOMS(J+1,IA)                                               LAP5 800
      VD1(J)=V1(J)                                                      LAP5 810
      DO 305 K=1,3                                                      LAP5 820
  305 QD(J,K)=Q(J,K)                                                    LAP5 830
      IF(VIEW)340,340,310                                               LAP5 840
C     ***** CALCULATE ENVELOPING CONE WITH ORIGIN AT VIEWPOINT *****   LAP5 850
  310 V1(3)=V1(3)-VIEW                                                  LAP5 860
      VD1(3)=V1(3)                                                      LAP5 870
C     ***** FORM COFACTOR MATRIX *****                                 LAP5 880
      DO 315 J=1,3                                                      LAP5 890
      J1=MOD(J,3)+1                                                     LAP5 900
      J2=MOD(J+1,3)+1                                                   LAP5 910
      DO 315 K=J,3                                                      LAP5 920
      K1=MOD(K,3)+1                                                     LAP5 930
      K2=MOD(K+1,3)+1                                                   LAP5 940
      QC(J,K)= QD(J1,K1)*QD(J2,K2)-QD(J1,K2)*QD(J2,K1)                  LAP5 950
  315 QC(K,J)=QC(J,K)                                                   LAP5 960
C     ***** FORM POLARIZED COFACTOR MATRIX AND ADD TO ELLIPSOID MATRIX *LAP5 970
      TD2=-SCL**2                                                       LAP5 980
C     ***** TD1 IS AN ARBITRARY SCALING FACTOR *****                   LAP5 990
      TD1=VMV(V1,Q,V1)                                                  LAP51000
      DO 325 J=1,3                                                      LAP51010
      J1=MOD(J,3)+1                                                     LAP51020
      J2=MOD(J+1,3)+1                                                   LAP51030
      DO 320 K=J,3                                                      LAP51040
      K1=MOD(K,3)+1                                                     LAP51050
      K2=MOD(K+1,3)+1                                                   LAP51060
      QD(J,K)=((VD1(J2)*(QC(J1,K1)*VD1(K2)-QC(J1,K2)*VD1(K1))           LAP51070
     1 +VD1(J1)*(VD1(K1)*QC(J2,K2)-VD1(K2)*QC(J2,K1)))+TD2*QD(J,K))/TD1 LAP51080
  320 QD(K,J)=QD(J,K)                                                   LAP51090
C     ***** PROJECTED ELLIPSE IN HOMOGENEOUS COORD OF WORKING SYSTEM ***LAP51100
      QD(J,3)=-QD(J,3)*VIEW                                             LAP51110
  325 QD(3,J)=-QD(3,J)*VIEW                                             LAP51120
C     ***** PROJECT CENTER OF ATOM ONTO PROJECTION PLANE *****         LAP51130
      TD1=-VIEW/VD1(3)                                                  LAP51140
      VD2(1)=VD1(1)*TD1                                                 LAP51150
      VD2(2)=VD1(2)*TD1                                                 LAP51160
C     ***** TRANSFORM TO NEW ORIGIN TO IMPROVE CONDITION OF MATRIX Q ***LAP51170
      DO 330 J=1,3                                                      LAP51180
      DO 330 K=1,2                                                      LAP51190
  330 QD(J,3)=QD(J,3)+QD(J,K)*VD2(K)                                    LAP51200
      DO 335 J=1,3                                                      LAP51210
      DO 335 K=1,2                                                      LAP51220
  335 QD(3,J)=QD(3,J)+VD2(K)*QD(K,J)                                    LAP51230
      V6(1)=XO(1)+VD2(1)                                                LAP51240
      V6(2)=XO(2)+VD2(2)                                                LAP51250
      GO TO 355                                                         LAP51260
C     ***** CALCULATE ENVELOPING CYLINDER ALONG Z OF WORKING SYSTEM ****LAP51270
  340 DO 345 J=1,2                                                      LAP51280
      DO 345 K=1,2                                                      LAP51290
  345 QD(J,K)=QD(J,K)-QD(J,3)*QD(K,3)/QD(3,3)                           LAP51300
      DO 350 J=1,2                                                      LAP51310
      QD(J,3)=0.0                                                       LAP51320
      QD(3,J)=0.0                                                       LAP51330
  350 V6(J)=XO(J)+ATOMS(J+1,IA)                                         LAP51340
C     ***** PROJECTED ELLIPSE IN HOMOGENEOUS COORD ABOUT CENTER OF ATOM LAP51350
      QD(3,3)=-SCL**2                                                   LAP51360
C     ***** FIT RECTANGLE AROUND ELLIPSE ALLOWING OVERLAP MARGIN *****  LAP51370
C     ***** FORM MATRIX OF COFACTORS *****                             LAP51380
  355 DO 360 J=1,3                                                      LAP51390
      J1=MOD(J,3)+1                                                     LAP51400
      J2=MOD(J+1,3)+1                                                   LAP51410
      DO 360 K=J,3                                                      LAP51420
      K1=MOD(K,3)+1                                                     LAP51430
      K2=MOD(K+1,3)+1                                                   LAP51440
  360 QC(J,K)= QD(J1,K1)*QD(J2,K2)-QD(J1,K2)*QD(J2,K1)                  LAP51450
C     ***** RESCALE MATRIX OF COFACTORS SO THAT QC(3,3)=1.0 *****      LAP51460
      DO 365 J=1,3                                                      LAP51470
      DO 365 K=J,3                                                      LAP51480
      QC(J,K)= QC(J,K)/QC(3,3)                                          LAP51490
  365 QC(K,J)=QC(J,K)                                                   LAP51500
      TD2=QD(3,3)                                                       LAP51510
      NDG=0                                                             LAP51520
      DO 385 J=1,2                                                      LAP51530
C     ***** SOLVE QUADRATIC EQUATION *****                             LAP51540
      T1 =QC(3,J)**2-QC(J,J)                                            LAP51550
      IF(T1)370,370,375                                                 LAP51560
C     ***** ROUNDOFF PROBLEMS, RESET LIMITS IN X OR Y *****            LAP51570
  370 NDG=1                                                             LAP51580
      V5(J)=0.001+OVMRGN                                                LAP51590
      GO TO 380                                                         LAP51600
  375 V5(J)=  SQRT(T1)+OVMRGN                                           LAP51610
      V6(J)=V6(J)+QC(3,J)                                               LAP51620
      TD2=TD2+QD(3,J)*QC(3,J)                                           LAP51630
  380 CONIC(2*J-1,IA)=V6(J)-V5(J)                                       LAP51640
  385 CONIC(2*J,IA)=V6(J)+V5(J)                                         LAP51650
      IF(NDG)390,390,395                                                LAP51660
  390 IF(TD2)400,395,395                                                LAP51670
C     ***** ELLIPSE IMAGINARY DUE TO ROUNDOFF, RESET TO REAL VALUE *****LAP51680
  395 CONIC(5,IA)=1.0/((CONIC(2,IA)-CONIC(1,IA))*0.5)**2                LAP51690
      CONIC(6,IA)=0.0                                                   LAP51700
      CONIC(7,IA)=1.0/((CONIC(4,IA)-CONIC(3,IA))*0.5)**2                LAP51710
      GO TO 405                                                         LAP51720
C     ***** STORE NORMALIZED QUADRATIC COEFFICIENTS FOR ELLIPSE *****  LAP51730
C     ***** SCALED BY OVERLAP MARGIN PARAMETER *****                   LAP51740
  400 TD3= -(1.0-2.0*OVMRGN/(V5(1)+V5(2)))**2 /TD2                      LAP51750
      CONIC(5,IA)=QD(1,1)*TD3                                           LAP51760
      CONIC(6,IA)=QD(1,2)*TD3                                           LAP51770
      CONIC(7,IA)=QD(2,2)*TD3                                           LAP51780
  405 CONTINUE                                                          LAP51790
      NCONIC=LATM                                                       LAP51800
C     ***** PRINT OUT SORTED ATOMS ARRAY *****                         LAP51810
      WRITE (NOUT,4)(ATOMS(1,J),J=1,LATM)                               LAP51820
    4 FORMAT(1H0,10X,30HCONTENTS OF SORTED ATOMS ARRAY/(15X,10F10.0))   LAP51830
C     ***** STORE BOND QUADRANGLES IF SEARCH CODES ARE GIVEN *****     LAP51840
      IF(NCD)420,420,410                                                LAP51850
C     ***** GENERATE PSEUDO-INSTRUCTION 822 TO CALCULATE BONDS *****   LAP51860
  410 NJ2=22                                                            LAP51870
      CALL P800                                                         LAP51880
      IF(NQUAD)420,420,415                                              LAP51890
C     ***** PRINT OUT NUMBER OF BOND QUADRANGLES STORED *****          LAP51900
C     ***** PRINT OUT QUADRANGLE IDENTIFICATION ARRAY *****            LAP51910
  415 WRITE (NOUT,6)NQUAD,(QUAD(9,J),J=1,NQUAD)                         LAP51920
    6 FORMAT(1H0,10X,27HBOND OVERLAP ARRAY CONTAINS,I4,23H BONDS (MAXIMULAP51930
     1M IS 599)/  11X,  66HATOM-PAIR NUMBERS IN ARRAY REFER TO SEQUENCE LAP51940
     2IN SORTED ATOMS ARRAY/(15X,10F10.0))                              LAP51950
  420 RETURN                                                            LAP51960
      END                                                               LAP51970


      SUBROUTINE LAP700(NA,ICQ)                                         LAP7  10
      DIMENSION DETER(2),QA(3,3,2),QC(3,3,2),V12(3,2),YMIN(2),YMAX(2)   LAP7  20
      DIMENSION OVMR(2)                                                 LAP7  30
C     ***** IN GENERAL, DOUBLE PRECISION IS NOT REQUIRED *****         LAP7  40
C     ***** BUT IN CASE OF TROUBLE, ACTIVATE THE CD COMMENT CARDS ***** LAP7  50
      REAL*8 AOV3,AOV3SQ,BOV3,DETER,PI,PHI,POV3,POV3CU,QA,QC,QOV2,QOV2SQLAP7  60
      REAL*8 ROOT,TD                                                    LAP7  70
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER, LAP7  80
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)         LAP7  90
      REAL*8 CHEM                                                       LAP7 100
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    LAP7 110
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)LAP7 120
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) LAP7 130
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAP7 140
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   LAP7 150
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   LAP7 160
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAP7 170
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   LAP7 180
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD LAP7 190
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAP7 200
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAP7 210
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                LAP7 220
      PI=3.1415926535897932                                             LAP7 230
CS    PI=3.141593                                                       LAP7 240
      ICQ=0                                                             LAP7 250
      NCOVER=0                                                          LAP7 260
      NQOVER=0                                                          LAP7 270
      OVMR(1)=OVMRGN                                                    LAP7 280
      OVMR(2)=0.0                                                       LAP7 290
      IF(NCONIC-NA)200,200,205                                          LAP7 300
  200 RETURN                                                            LAP7 310
C     ***** ROUGH CHECK FOR OVERLAPPING ATOMS *****                    LAP7 320
  205 DO  210 J=1,2                                                     LAP7 330
      YMIN(J)=CONIC(2*J-1,NA)                                           LAP7 340
  210 YMAX(J)=CONIC(2*J,NA)                                             LAP7 350
      L=0                                                               LAP7 360
      DO 420 IA=NA,NCONIC                                               LAP7 370
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      IF(IA-NA)230,230,215                                              LAP7 380
  215 DO 225 J=1,2                                                      LAP7 390
      IF(YMAX(J)-CONIC(2*J-1,IA))420,420,220                            LAP7 400
  220 IF(YMIN(J)-CONIC(2*J,IA))225,420,420                              LAP7 410
  225 CONTINUE                                                          LAP7 420
C     ***** EXACT CHECK FOR OVERLAPPING ATOMS *****                     LAP7 430
  230 IF(L-1)235,235,240                                                LAP7 440
  235 L=L+1                                                             LAP7 450
  240 CALL LAPCON(CONIC(1,IA),DA,V12(1,L),OVMR(L))                      LAP7 460
      DO 245 J=1,3                                                      LAP7 470
      DO 245 K=1,3                                                      LAP7 480
  245 QA(J,K,L)=DA(J,K)                                                 LAP7 490
C     ***** CALCULATE COFACTORS AND DETERMINANTS *****                  LAP7 500
      DETER(L)=0.0                                                      LAP7 510
      DO 250 J=1,3                                                      LAP7 520
      J1=MOD(J+3,3)+1                                                   LAP7 530
      J2=MOD(J+1,3)+1                                                   LAP7 540
      DO 250 K=1,3                                                      LAP7 550
      K1=MOD(K+3,3)+1                                                   LAP7 560
      K2=MOD(K+1,3)+1                                                   LAP7 570
      TD=QA(J1,K1,L)*QA(J2,K2,L)-QA(J1,K2,L)*QA(J2,K1,L)                LAP7 580
      DETER(L)=DETER(L)+TD*QA(J,K,L)                                    LAP7 590
  250 QC(J,K,L)=TD                                                      LAP7 600
C     ***** DETER(L) IS THE DETERMINANT TIMES 3 *****                   LAP7 610
      IF(L-1)420,420,255                                                LAP7 620
C     ***** FORM CHARACTERISTIC EQUATION AND EXAMINE ITS ROOTS *****    LAP7 630
  255 AOV3=0.0                                                          LAP7 640
      BOV3=0.0                                                          LAP7 650
      DO 260 J=1,3                                                      LAP7 660
      DO 260 K=1,3                                                      LAP7 670
      AOV3=AOV3+QC(J,K,2)*QA(J,K,1)                                     LAP7 680
  260 BOV3=BOV3+QC(J,K,1)*QA(J,K,2)                                     LAP7 690
      AOV3=AOV3/ DETER(2)                                               LAP7 700
      AOV3SQ=AOV3**2                                                    LAP7 710
      BOV3=BOV3/ DETER(2)                                               LAP7 720
      POV3=BOV3-AOV3SQ                                                  LAP7 730
      QOV2=AOV3*(AOV3SQ-BOV3*1.5D0)+DETER(1)/(DETER(2)*2.0D0)           LAP7 740
CS    QOV2=AOV3*(AOV3SQ-BOV3*1.5  )+DETER(1)/(DETER(2)*2.0  )           LAP7 750
C     ***** CHECK DISCRIMINANT OF CHARACTERISTIC CUBIC EQUATION *****   LAP7 760
      ITYPE=0                                                           LAP7 770
      POV3CU=POV3**3                                                    LAP7 780
      QOV2SQ=QOV2**2                                                    LAP7 790
      IF(POV3CU+QOV2SQ)270,310,265                                      LAP7 800
  265 IF(POV3CU*1.00001 +QOV2SQ)310,310,400                             LAP7 810
  270 IF(POV3CU+1.00001 *QOV2SQ)275,310,310                             LAP7 820
C     ***** THREE REAL ROOTS, ALL DIFFERENT *****                       LAP7 830
  275 ITYPE=1                                                           LAP7 840
C     ***** NO INTERSECTION IF A/3 AND B/3 INVARIANTS ARE NEGATIVE *****LAP7 850
      IF(AOV3)280,285,285                                               LAP7 860
  280 IF(BOV3)420,285,285                                               LAP7 870
C     ***** CALCULATE ONE ROOT OF CHARACTERISTIC CUBIC EQUATION *****   LAP7 880
  285 IF(QOV2)295,290,295                                               LAP7 890
  290 PHI=PI/2.0D0                                                      LAP7 900
CS290 PHI=PI/2.0                                                        LAP7 910
      GO TO 305                                                         LAP7 920
  295 PHI=DATAN(-DSQRT(-POV3CU-QOV2SQ)/QOV2)                            LAP7 930
CS295 PHI= ATAN(- SQRT(-POV3CU-QOV2SQ)/QOV2)                            LAP7 940
      IF(PHI)300,305,305                                                LAP7 950
  300 PHI=PHI+PI                                                        LAP7 960
  305 ROOT=2.0D0*DSQRT(-POV3)*DCOS(PHI/3.0D0)-AOV3                      LAP7 970
CS305 ROOT=2.0  * SQRT(-POV3)* COS(PHI/3.0  )-AOV3                      LAP7 980
      GO TO 325                                                         LAP7 990
C     ***** THREE REAL ROOTS, AT LEAST TWO ARE EQUAL *****              LAP71000
  310 ITYPE=2                                                           LAP71010
C     ***** CHECK SIGNS OF INVARIANTS A/3 AND B/3 *****                 LAP71020
      IF(AOV3)315,320,320                                               LAP71030
  315 IF(BOV3)420,320,320                                               LAP71040
C     ***** CALCULATE REPEATED RCOT OF CUBIC EQUATION *****             LAP71050
  320 ROOT=DSIGN(DSQRT(-POV3),QOV2)-AOV3                                LAP71060
CS320 ROOT= SIGN( SQRT(-POV3),QOV2)-AOV3                                LAP71070
C     ***** FORM DEGENERATE CONIC (LINE PAIR WHICH MAY BE COINCIDENT) **LAP71080
  325 DO 330 J=1,3                                                      LAP71090
      DO 330 K=1,3                                                      LAP71100
  330 DA(J,K)=QA(J,K,1)+ROOT*QA(J,K,2)                                  LAP71110
C     ***** EXAMINE INVARIANTS OF THE DEGENERATE CONIC *****            LAP71120
      T6=DA(1,1)*DA(2,2)                                                LAP71130
      T7=DA(1,2)**2                                                     LAP71140
C     ***** NEGATIVE DENOTES REAL INTERSECTING LINE PAIR *****          LAP71150
C     ***** POSITIVE DENOTES IMAGINARY LINES INTERSECTING AT REAL POINT LAP71160
      IF(T6-T7)335,345,340                                              LAP71170
  335 IF(T6*1.0001  -T7)400,345,345                                     LAP71180
  340 IF(T6-1.0001  *T7)345,345,365                                     LAP71190
  345 T8=DA(3,3)*(DA(1,1)+DA(2,2))                                      LAP71200
      T9=DA(1,3)**2+DA(2,3)**2                                          LAP71210
C     ***** NEGATIVE DENOTES REAL PARALLEL LINE PAIR *****              LAP71220
C     ***** POSITIVE DENOTES IMAGINARY PARALLELS *****                  LAP71230
C     ***** ZERO DENOTES ONE REAL LINE (COINCIDENT PARALLELS) *****     LAP71240
      IF(T8-T9)350,360,355                                              LAP71250
  350 IF(T8*1.0001  -T9)400,360,360                                     LAP71260
  355 IF(T8-1.0001  *T9)360,360,365                                     LAP71270
C     ***** COINCIDENT LINE PAIR FOUND FOR THE REPEATED ROOT *****      LAP71280
  360 ITYPE=3                                                           LAP71290
C     ***** COMPARE AREAS OF CONICS *****                               LAP71300
  365 KA=1                                                              LAP71310
      KB=2                                                              LAP71320
      IF(QC(3,3,KA)-QC(3,3,KB))370,375,375                              LAP71330
  370 KA=2                                                              LAP71340
      KB=1                                                              LAP71350
C     ***** SEE IF ONE CONIC IS INSIDE THE OTHER CONIC *****            LAP71360
  375 T1=0.0                                                            LAP71370
      DO 385 J=1,3                                                      LAP71380
      T2=QA(J,3,KB)                                                     LAP71390
      DO 380 K=1,2                                                      LAP71400
  380 T2=T2+QA(J,K,KB)*V12(K,KA)                                        LAP71410
  385 T1=T1+V12(J,KA)*T2                                                LAP71420
C     ***** DISCARD IF KA IS OUTSIDE KB *****                           LAP71430
      IF(T1)390,390,420                                                 LAP71440
  390 IF(KA-1)395,395,400                                               LAP71450
C     ***** THE OVERLAPPING ATOM HIDES THE ORIGINAL ATOM *****          LAP71460
  395 ICQ=-1                                                            LAP71470
      RETURN                                                            LAP71480
C     ***** STORE OVERLAPPING ATOM *****                                LAP71490
  400 ICQ=ICQ+1                                                         LAP71500
      IF(NCOVER-20)410,405,405                                          LAP71510
  405 NG=17                                                             LAP71520
      CALL ERPNT(ATOMS(1,IA),700)                                       LAP71530
      NCOVER=NCOVER-1                                                   LAP71540
  410 NCOVER=NCOVER+1                                                   LAP71550
      IJ=1                                                              LAP71560
      DO 415 I=1,3                                                      LAP71570
      DO 415 J=I,3                                                      LAP71580
      COVER(IJ,NCOVER)=QA(I,J,2)                                        LAP71590
  415 IJ=IJ+1                                                           LAP71600
      KC(NCOVER)=IA                                                     LAP71610
  420 CONTINUE                                                          LAP71620
C     ***** SECOND PART OF SUBROUTINE CHECKS FOR BONDS OVER THE ATOM ***LAP71630
  425 IF(NQUAD)470,470,430                                              LAP71640
  430 ITY=0                                                             LAP71650
C     ***** ROUGH CHECK FOR OVERLAPPING BONDS *****                     LAP71660
      DO 465 IQ=1,NQUAD                                                 LAP71670
      TID=QUAD(9,IQ)                                                    LAP71680
      NA1=TID/1000.                                                     LAP71690
      NA2=AMOD(TID,1000.)                                               LAP71700
      IF(NA-NA2)435,435,465                                             LAP71710
  435 DO 445 J=1,2                                                      LAP71720
      IF(YMAX(J)-AMIN1(QUAD(J,IQ),QUAD(J+2,IQ),QUAD(J+4,IQ),QUAD(J+6,IQ)LAP71730
     1 ))465,465,440                                                    LAP71740
  440 IF(YMIN(J)-AMAX1(QUAD(J,IQ),QUAD(J+2,IQ),QUAD(J+4,IQ),QUAD(J+6,IQ)LAP71750
     1 ))445,465,465                                                    LAP71760
  445 CONTINUE                                                          LAP71770
C     ***** EXACT CHECK FOR OVERLAPPING BONDS *****                     LAP71780
  450 ITY=ITY-1                                                         LAP71790
      IQQ=0                                                             LAP71800
      CALL LAPAB(IQ,NA,IQQ,ITY)                                         LAP71810
      IF(IQQ)455,460,460                                                LAP71820
  455 ICQ=-1                                                            LAP71830
      RETURN                                                            LAP71840
  460 ICQ=ICQ+1                                                         LAP71850
      IF(NQOVER-30)465,470,470                                          LAP71860
  465 CONTINUE                                                          LAP71870
  470 RETURN                                                            LAP71880
      END                                                               LAP71890
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      SUBROUTINE LAP800(NA1,NA2,ICQ)                                    LAP8  10
C     ***** SUBROUTINE CHECKS FOR ATOMS AND BONDS OVERLAPPING A BOND ***LAP8  20
      DIMENSION FL(4,4),Y1(2),Y2(2),YMAX(2),YMIN(2),QUA(3,4)            LAP8  30
      DIMENSION VUE(3)                                                  LAP8  40
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER, LAP8  50
     1 NCOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)         LAP8  60
      REAL*8 CHEM                                                       LAP8  70
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    LAP8  80
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)LAP8  90
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) LAP8 100
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAP8 110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   LAP8 120
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   LAP8 130
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAP8 140
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      COMMON NG,A,AA,AAREV,AAWBK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   LAP8 150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD LAP8 160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REPV,RES,RMS,SCAL1LAP8 170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAP8 180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                LAP8 190
      IQ=0                                                              LAP8 200
      ICQ=0                                                             LAP8 210
      IF(NA1*NA2)245,245,195                                            LAP8 220
  195 TID1=FLOAT(NA1)*1000.+FLOAT(NA2)                                  LAP8 230
      IF(NCONIC)245,245,200                                             LAP8 240
  200 IF(NJ2-21)250,205,205                                             LAP8 250
C     ***** PART 1, CALLED FROM BOND, STORES BOND OUTLINE INFORMATION **LAP8 260
  205 IF(NQUAD-599)215,210,210                                          LAP8 270
  210 NG=16                                                             LAP8 280
      CALL ERPNT(ATOMS(1,NA1),822)                                      LAP8 290
      GO TO 245                                                         LAP8 300
  215 NQUAD=NQUAD+1                                                     LAP8 310
C     ***** CALCULATE OVERLAP MARGIN FOR BOND QUADRANGLE *****          LAP8 320
      T1=0.0                                                            LAP8 330
      T2=0.0                                                            LAP8 340
      DO 220 J=1,2                                                      LAP8 350
      Y1(J)=DP(J,1)-DP(J,65)                                            LAP8 360
      Y2(J)=DP(J,2)-DP(J,66)                                            LAP8 370
      T1=T1+Y1(J)**2                                                    LAP8 380
  220 T2=T2+Y2(J)**2                                                    LAP8 390
      IF(T1*T2)225,225,230                                              LAP8 400
  225 T1=0.0                                                            LAP8 410
      T2=0.0                                                            LAP8 420
      GO TO 235                                                         LAP8 430
  230 T1=OVMRGN/SQRT(T1)                                                LAP8 440
      T2=OVMRGN/SQRT(T2)                                                LAP8 450
C     ***** STORE BOND QUADRANGLE *****                                 LAP8 460
  235 DO 240 J=1,2                                                      LAP8 470
      Y1(J)=Y1(J)*T1                                                    LAP8 480
      Y2(J)=Y2(J)*T2                                                    LAP8 490
      QUAD(J,NQUAD)=DP(J,1)+Y1(J)                                       LAP8 500
      QUAD(J+2 ,NQUAD)=DP(J,2)+Y2(J)                                    LAP8 510
      QUAD(J+4,NQUAD)=DP(J,66)-Y2(J)                                    LAP8 520
  240 QUAD(J+6,NQUAD)=DP(J,65)-Y1(J)                                    LAP8 530
      QUAD(9,NQUAD)=TID1                                                LAP8 540
  245 RETURN                                                            LAP8 550
C     ***** PART 2, CALLED FROM BOND, OVERLAP CHECK FOR BOND NA1-NA2 ***LAP8 560
  250 NCOVER=0                                                          LAP8 570
      NQOVER=0                                                          LAP8 580
      TOL=1.E-5                                                         LAP8 590
      IF(NCONIC-NA1)245,245,255                                         LAP8 600
C     ***** SAVE QUADRANGLE TEMPORARILY *****                           LAP8 610
  255 IQ=NQUAD+1                                                        LAP8 620
      DO 260 J=1,2                                                      LAP8 630
      QUAD(J,IQ)=DP(J,1)                                                LAP8 640
      QUAD(J+2,IQ)=DP(J,2)                                              LAP8 650
      QUAD(J+4,IQ)=DP(J,66)                                             LAP8 660
  260 QUAD(J+6,IQ)=DP(J,65)                                             LAP8 670
      QUAD(9,IQ)=TID1                                                   LAP8 680
C     ***** FIT RECTANGLE AROUND QUADRANGLE *****                       LAP8 690
  265 DO 270 J=1,2                                                      LAP8 700
      YMIN(J)=AMIN1(DP(J,1),DP(J,2),DP(J,66),DP(J,65))                  LAP8 710
  270 YMAX(J)=AMAX1(DP(J,1),DP(J,2),DP(J,66),DP(J,65))                  LAP8 720
C     ***** ROUGH CHECK FOR ATOM-OVER-BOND OVERLAP *****                LAP8 730
      NA1P1=NA1+1                                                       LAP8 740
      ITY=0                                                             LAP8 750
      DO 305 IA=NA1P1,NCONIC                                            LAP8 760
      DO 285 J=1,2                                                      LAP8 770
      IF(IA-NA2)275,305,275                                             LAP8 780
  275 IF(YMAX(J)-CONIC(2*J-1,IA))305,305,280                            LAP8 790
  280 IF(YMIN(J)-CONIC(2*J,IA))285,305,305                              LAP8 800
  285 CONTINUE                                                          LAP8 810
C     ***** CHECK FOR TRUE ATOM-OVER-BOND OVERLAP *****                 LAP8 820
      ITY=ITY+1                                                         LAP8 830
      CALL LAPAB(IQ,IA,IQQ,ITY)                                         LAP8 840
      IF(IQQ)290,305,300                                                LAP8 850
C     ***** HIDDEN BOND *****                                           LAP8 860
  290 ICQ=-1                                                            LAP8 870
  295 RETURN                                                            LAP8 880
  300 ICQ=ICQ+1                                                         LAP8 890
      IF(NCOVER-20)305,310,310                                          LAP8 900
  305 CONTINUE                                                          LAP8 910
  310 IF(NQUAD)295,295,315                                              LAP8 920
C     ***** ROUGH CHECK FOR BOND-OVER-BOND OVERLAP *****                LAP8 930
  315 CALL DIFV(ATOMS(2,NA2),ATOMS(2,NA1),V1)                           LAP8 940
      CALL UNIT(V1,V1,1)                                                LAP8 950
      VUE(1)=  ATOMS(2,NA1)                                             LAP8 960
      VUE(2)=  ATOMS(3,NA1)                                             LAP8 970
      VUE(3)=  ATOMS(4,NA1)-VIEW                                        LAP8 980
      DO 495 IB=1,NQUAD                                                 LAP8 990
      TID2=QUAD(9,IB)                                                   LAP81000
      IF(TID1-TID2)320,495,320                                          LAP81010
  320 NB2=AMOD(TID2,1000.)                                              LAP81020
      NB1=TID2/1000.                                                    LAP81030
      IF(NA1-NB2)325,495,495                                            LAP81040
  325 DO 335 J=1,2                                                      LAP81050
      IF(YMAX(J)-AMIN1(QUAD(J,IB),QUAD(J+2,IB),QUAD(J+4,IB),QUAD(J+6,IB)LAP81060
     1 ))495,495,330                                                    LAP81070
  330 IF(YMIN(J)-AMAX1(QUAD(J,IB),QUAD(J+2,IB),QUAD(J+4,IB),QUAD(J+6,IB)LAP81080
     1 ))335,495,495                                                    LAP81090
  335 CONTINUE                                                          LAP81100
C     ***** SET UP LINEAR FORMS FOR EDGES OF QUADRANGLE *****           LAP81110
      DO 345 L=1,4                                                      LAP81120
      K=2*L                                                             LAP81130
      K1=MOD(K,8)+2                                                     LAP81140
      QUA(1,L)=QUAD(K,IB)-QUAD(K1,IB)                                   LAP81150
      QUA(2,L)=QUAD(K1-1,IB)-QUAD(K-1,IB)                               LAP81160
      QUA(3,L)=QUAD(K-1,IB)*QUAD(K1,IB)-QUAD(K,IB)*QUAD(K1-1,IB)        LAP81170
C     ***** NORMALIZE LINE EQUATION COEFFICIENTS *****                  LAP81180
      T1=SQRT(QUA(1,L)**2+QUA(2,L)**2)                                  LAP81190
      IF(T1)495,495,340                                                 LAP81200
  340 DO 345 J=1,3                                                      LAP81210
  345 QUA(J,L)=QUA(J,L)/T1                                              LAP81220
C     ***** EVALUATE LINEAR FORMS AND SIGNATURES FOR QUADRANGLE *****   LAP81230
      T3=3.0                                                            LAP81240
      DO 365 K=1,4                                                      LAP81250
      T2=3.0                                                            LAP81260
      J=K*2                                                             LAP81270
      DO 355 L=1,4                                                      LAP81280
      T1=QUAD(J-1,IQ)*QUA(1,L)+QUAD(J,IQ)*QUA(2,L)+QUA(3,L)             LAP81290
      IF(T1)350,355,355                                                 LAP81300
  350 T2=T2-1.0                                                         LAP81310
  355 FL(L,K)=T1                                                        LAP81320
      IF(T2)360,365,365                                                 LAP81330
  360 T3=T3-1.0                                                         LAP81340
  365 CONTINUE                                                          LAP81350
C     ***** CHECK FOR 4 POINTS INSIDE QUADRANGLE *****                  LAP81360
      IF(T3)370,375,375                                                 LAP81370
  370 ITYPE=-1                                                          LAP81380
      GO TO 415                                                         LAP81390
C     ***** CHECK FOR 1 TO 3 POINTS INSIDE QUADRANGLE ****              LAP81400
  375 IF(T3-3.0)380,385,385                                             LAP81410
  380 ITYPE=0                                                           LAP81420
      GO TO 415                                                         LAP81430
C     ***** DETERMINE WHICH EDGES ARE CROSSED BY THE 4 LINE SEGMENTS ***LAP81440
  385 DO 405 L=1,4                                                      LAP81450
      L1=MOD(L,4)+1                                                     LAP81460
C     ***** LINE SEGMENT L FROM POINT Y1 TO POINT Y2 *****              LAP81470
      Y1(1)=QUAD(L*2-1,IQ)                                              LAP81480
      Y1(2)=QUAD(L*2,IQ)                                                LAP81490
      Y2(1)=QUAD(L1*2-1,IQ)                                             LAP81500
      Y2(2)=QUAD(L1*2,IQ)                                               LAP81510
      DO 405 K=1,4                                                      LAP81520
      T1=FL(K,L)                                                        LAP81530
      T2=FL(K,L1)                                                       LAP81540
      T3=T1-T2                                                          LAP81550
C     ***** T1 AND T2 MUST HAVE OPPOSITE SIGNS FOR INTERSECTION TO OCCURLAP81560
      IF(T1*T2)390,390,405                                              LAP81570
C     ***** COMPONENT OF SEGMENT L PERPENDICULAR TO EDGE K OF IB IS T3  LAP81580
  390 IF(ABS(T3)-1.E-5)405,405,395                                      LAP81590
C     ***** CALCULATE COORDINATES OF INTERSECTION *****                 LAP81600
  395 T4=(T1*Y2(1)-T2*Y1(1))/T3                                         LAP81610
      T5=(T1*Y2(2)-T2*Y1(2))/T3                                         LAP81620
      K0=2*K                                                            LAP81630
      K1=2*(MOD(K,4)+1)                                                 LAP81640
C     ***** IS INTERSECTION WITHIN QUADRANGLE IQ *****                  LAP81650
      T6=(T4-QUAD(K0-1,IB))*(QUAD(K1-1,IB)-T4)+(T5-QUAD(K0,IB))*        LAP81660
     1 (QUAD(K1,IB)-T5)                                                 LAP81670
      IF(ABS(T6)-1.E-4)410,410,400                                      LAP81680
  400 IF(T6)405,410,410                                                 LAP81690
  405 CONTINUE                                                          LAP81700
      GO TO 495                                                         LAP81710
  410 ITYPE=1                                                           LAP81720
C     ***** CHECK OVER/UNDER AMBIGUITY *****                            LAP81730
  415 IF((NA1-NB1)*(NA2-NB2)*(NA2-NB1))425,420,425                      LAP81740
C     ***** BONDS SHARE AN ATOM *****                                   LAP81750
  420 IF(NA1+NA2-NB1-NB2)465,495,495                                    LAP81760
  425 CALL DIFV(ATOMS(2,NB2),ATOMS(2,NB1),V2)                           LAP81770
      CALL DIFV(ATOMS(2,NB1),ATOMS(2,NA1),V4)                           LAP81780
      CALL UNIT(V2,V2,1)                                                LAP81790
      CALL UNIT(V4,V4,1)                                                LAP81800
      CALL NORM(V1,V2,V3,1)                                             LAP81810
      IF(VV(V3,V3)-TOL)430,430,435                                      LAP81820
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C     ***** PARALLEL BONDS, RECALCULATE V3 *****                        LAP81830
  430 CALL NORM(V1,V4,V5,1)                                              LAP81840
      CALL NORM(V5,V1,V3,1)                                              LAP81850
C     ***** CHECK FOR COLLINEAR BONDS *****                             LAP81860
      IF(VV(V3,V3)-TOL)465,465,450                                       LAP81870
  435 IF(VV(V3,V4)+TOL)440,450,450                                       LAP81880
  440 DO 445 J=1,3                                                       LAP81890
  445 V3(J)=-V3(J)                                                       LAP81900
C     ***** V3 IS NORMAL TO BONDS IQ AND IB GOING FROM IQ TOWARD IB ***  LAP81910
  450 IF(VIEW)455,455,460                                                LAP81920
  455 IF(V3(3))495,495,465                                               LAP81930
  460 IF(VV(VUE,V3))465,495,495                                          LAP81940
C     ***** OVERLAPPING BOND FOUND *****                                LAP81950
  465 ICQ=ICQ+1                                                          LAP81960
      IF(ITYPE)470,475,475                                               LAP81970
C     ***** HIDDEN BOND *****                                           LAP81980
  470 ICQ=-1                                                             LAP81990
      RETURN                                                             LAP82000
C     ***** STORE INTERFERING QUADRANGLE *****                          LAP82010
  475 IF(NQOVER-30)485,480,480                                           LAP82020
  480 NG=17                                                              LAP82030
      CALL ERPNT(TID2,800)                                               LAP82040
      RETURN                                                             LAP82050
  485 NQOVER=NQOVER+1                                                    LAP82060
      DO 490 K=1,4                                                       LAP82070
      DO 490 J=1,3                                                       LAP82080
  490 QOVER(J,K,NQOVER)=QUA(J,K)                                         LAP82090
      KQ(NQOVER)=IB                                                      LAP82100
  495 CONTINUE                                                           LAP82110
  500 RETURN                                                             LAP82120
      END                                                                LAP82130


      SUBROUTINE LAPAB(IQ,IA,ICQ,ITY)                                    LAPA  10
C     ***** SUBROUTINE CHECKS FOR OVERLAP BETWEEN ATOMS AND BONDS *****  LAPA  20
C     ***** CALLED BY SUBROUTINES LAP700 AND LAP800 *****               LAPA  30
      DIMENSION BF(4),CON(3,3),QF(5),QUA(3,4)                            LAPA  40
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER,  LAPA  50
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)          LAPA  60
      REAL*8 CHEM                                                        LAPA  70
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)     LAPA  80
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) LAPA  90
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)  LAPA 100
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  LAPA 110
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)    LAPA 120
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    LAPA 130
      DIMENSION XLNG(3),XO(3),XT(3)                                      LAPA 140
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D    LAPA 150
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,IATM,LINO,NATOM,NCD  LAPA 160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAPA 170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    LAPA 180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                 LAPA 190
      TID=QUAD(9,IQ)                                                     LAPA 200
      NA1=TID/1000.                                                      LAPA 210
      NA2=AMOD(TID,1000.)                                                LAPA 220
C     ***** ITY.GT.0, CHECK FOR ATOMS OVER A BOND ****                  LAPA 230
C     ***** ITY.LT.0, CHECK FOR BONDS OVER AN ATOM *****                LAPA 240
      ICQ=0                                                              LAPA 250
      IF(ITY)210,200,205                                                 LAPA 260
  200 RETURN                                                             LAPA 270
  205 CALL LAPCON(CONIC(1,IA),CON,V1,0.0)                                LAPA 280
      IF(ITY-2)220,240,240                                               LAPA 290
  210 IF(ITY+2)220,220,215                                               LAPA 300
  215 CALL LAPCON(CONIC(1,IA),CON,V1,OVMRGN)                             LAPA 310
C     ***** SET UP LINEAR FORMS FOR EDGES OF QUADRANGLE *****           LAPA 320
  220 DO 235 L=1,4                                                       LAPA 330
      K=2*L                                                              LAPA 340
      K1=MOD(K,8)+2                                                      LAPA 350
      QUA(1,L)=QUAD(K,IQ)-QUAD(K1,IQ)                                    LAPA 360
      QUA(2,L)=QUAD(K1-1,IQ)-QUAD(K-1,IQ)                                LAPA 370
      QUA(3,L)=QUAD(K-1,IQ)*QUAD(K1,IQ)-QUAD(K,IQ)*QUAD(K1-1,IQ)         LAPA 380
      T1=SQRT(QUA(1,L)**2+QUA(2,L)**2)                                   LAPA 390
      IF(T1)225,225,230                                                  LAPA 400
  225 ITY=0                                                              LAPA 410
      ICQ=0                                                              LAPA 420
      GO TO 430                                                          LAPA 430
C     ***** TRANSFORM COEFFICIENTS FOR EDGES TO NORMAL FORM *****       LAPA 440
  230 DO 235 J=1,3                                                       LAPA 450
  235 QUA(J,L)=QUA(J,L)/T1                                               LAPA 460
C     ***** EVALUATE 4 QUADRATIC AND 4 BILINEAR FORMS *****             LAPA 470
  240 V2(3)=1.0                                                          LAPA 480
      V3(3)=1.0                                                          LAPA 490
      T2=3.0                                                             LAPA 500
      DO 265 L=1,4                                                       LAPA 510
      L1=(MOD(L,4)+1)*2                                                  LAPA 520
      V2(1)=QUAD(2*L-1,IQ)                                               LAPA 530
      V2(2)=QUAD(2*L,IQ)                                                 LAPA 540
      V3(1)=QUAD(L1-1,IQ)                                                LAPA 550
      V3(2)=QUAD(L1,IQ)                                                  LAPA 560
      QF(L)=0.0                                                          LAPA 570
      BF(L)=0.0                                                          LAPA 580
      DO 250 K=1,3                                                       LAPA 590
      T1=CON(3,K)                                                        LAPA 600
      DO 245 J=1,2                                                       LAPA 610
  245 T1=T1+V2(J)*CON(J,K)                                               LAPA 620
      QF(L)=QF(L)+T1*V2(K)                                               LAPA 630
  250 BF(L)=BF(L)+T1*V3(K)                                               LAPA 640
      IF(QF(L))260,255,265                                               LAPA 650
  255 T2=T2-0.8                                                          LAPA 660
      GO TO 265                                                          LAPA 670
  260 T2=T2-1.0                                                          LAPA 680
  265 CONTINUE                                                           LAPA 690
      QF(5)=QF(1)                                                        LAPA 700
C     ***** CHECK FOR 4 POINTS OF QUADRANGLE INSIDE OR ON ELLIPSE ***** LAPA 710
      IF(T2)270,275,275                                                  LAPA 720
  270 ITYPE=-1                                                           LAPA 730
      GO TO 330                                                          LAPA 740
C     ***** CHECK FOR 1 TO 3 POINTS OF QUADRANGLE INSIDE THE ELLIPSE ***LAPA 750
  275 IF(T2-2.2)280,285,285                                              LAPA 760
  280 ITYPE=0                                                            LAPA 770
      IF(NA2-IA)340,375,335                                              LAPA 780
C     ***** CHECK FOR QUADRANGLE-ELLIPSE INTERSECTION *****             LAPA 790
  285 DO 305 K=1,4                                                       LAPA 800
C     ***** EVALUATE DISCRIMINANT *****                                 LAPA 810
      T1=BF(K)**2-QF(K)*QF(K+1)                                          LAPA 820
      IF(T1)305,305,290                                                  LAPA 830
  290 T1=SQRT(T1)                                                        LAPA 840
C     ***** IS INTERSECTION WITHIN BOUNDS OF QUADRANGLE *****           LAPA 850
      T3=QF(K)-BF(K)                                                     LAPA 860
      T4=T3+QF(K+1)-BF(K)                                                LAPA 870
      IF(ABS(T4)-1.E-5)305,305,295                                       LAPA 880
  295 T5=(T3-T1)/T4                                                      LAPA 890
      IF(T5)305,280,300                                                  LAPA 900
  300 IF(1.0-T5)305,305,280                                              LAPA 910
  305 CONTINUE                                                           LAPA 920
C     ***** NO VALID INTERSECTION FOUND *****                           LAPA 930
C     ***** CHECK FOR CENTER OF ELLIPSE WITHIN THE QUADRANGLE ****      LAPA 940
      T3=3.0                                                             LAPA 950
      DO 320 K=1,4                                                       LAPA 960
      T1=QUA(3,K)                                                        LAPA 970
      DO 310 J=1,2                                                       LAPA 980
  310 T1=T1+V1(J)*QUA(J,K)                                               LAPA 990
      IF(T1)315,320,320                                                  LAPA1000
  315 T3=T3-1.0                                                          LAPA1010
  320 CONTINUE                                                           LAPA1020
      IF(T3)325,370,370                                                  LAPA1030
  325 ITYPE=1                                                            LAPA1040
C     ***** CHECK OVER/UNDER AMBIGUITY *****                            LAPA1050
  330 IF(NA2-IA)375,375,335                                              LAPA1060
  335 IF(IA-NA1)375,375,340                                              LAPA1070
  340 CALL DIFV(ATOMS(2,NA2),ATOMS(2,NA1),V2)                            LAPA1080
      CALL DIFV(ATOMS(2,IA),ATOMS(2,NA1),V3)                             LAPA1090
      CALL UNIT(V2,V2,1)                                                 LAPA1100
      CALL UNIT(V3,V3,1)                                                 LAPA1110
      CALL NORM(V2,V3,V4,1)                                              LAPA1120
      IF(VV(V4,V4)-1.E-5)345,345,350                                     LAPA1130
C     ***** CENTER OF ATOM IQ IS ON THE BOND LINE *****                 LAPA1140
  345 IF(ITY)370,370,385                                                 LAPA1150
C     ***** CENTER OF ATOM IQ IS NOT ON THE BOND LINE *****             LAPA1160
  350 CALL NORM(V4,V2,V5,1)                                              LAPA1170
      T1=-V5(3)                                                          LAPA1180
      IF(VIEW)365,365,355                                                LAPA1190
  355 T1=V5(3)*(ATOMS(4,IA)-VIEW)                                        LAPA1200
      DO 360 J=1,2                                                       LAPA1210
  360 T1=T1+V5(J)*ATOMS(J+1,IA)                                          LAPA1220
  365 IF(T1*FLOAT(ITY))375,375,370                                       LAPA1230
C     ***** NO INTERFERENCE FOUND *****                                 LAPA1240
  370 ICQ=0                                                              LAPA1250
      GO TO 430                                                          LAPA1260
C     ***** ITYPE=1 ENCLOSED ELLIPSE / ITYPE=-1 ENCLOSED QUADRANGLE ****LAPA1270
  375 IF(ITYPE*ITY)380,385,385                                           LAPA1280
C     ***** HIDDEN ATOM OR HIDDEN BOND *****                            LAPA1290
  380 ICQ=-1                                                             LAPA1300
      GO TO 430                                                          LAPA1310
  385 ICQ=1                                                              LAPA1320
      IF(ITY)410,390,390                                                 LAPA1330
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C     ***** STORE INTERFERING ELLIPSE *****                              LAPA1340
  390 IF(NCOVER-20)400,395,395                                            LAPA1350
  395 NG=17                                                               LAPA1360
      CALL ERPNT(ATOMS(1,IA),800)                                         LAPA1370
      NCOVER=NCOVER-1                                                     LAPA1380
  400 NCOVER=NCOVER+1                                                     LAPA1390
      IJ=1                                                                LAPA1400
      DO 405 I=1,3                                                        LAPA1410
      DO 405 J=I,3                                                        LAPA1420
      COVER(IJ,NCOVER)=CON(I,J)                                           LAPA1430
  405 IJ=IJ+1                                                             LAPA1440
      KC(NCOVER)=IA                                                       LAPA1450
      GO TO 430                                                           LAPA1460
C     ***** STORE INTERFERING QUADRANGLE *****                            LAPA1470
  410 IF(NQOVER-30)420,415,415                                            LAPA1480
  415 NG=18                                                               LAPA1490
      CALL ERPNT(TID,700)                                                 LAPA1500
      NQOVER=NQOVER-1                                                     LAPA1510
  420 NQOVER=NQOVER+1                                                     LAPA1520
      DO 425 K=1,4                                                        LAPA1530
      DO 425 J=1,3                                                        LAPA1540
  425 QOVER(J,K,NQOVER)=QUA(J,K)                                          LAPA1550
      KQ(NQOVER)=IQ                                                       LAPA1560
  430 RETURN                                                              LAPA1570
      END                                                                 LAPA1580


      SUBROUTINE LAPCON(CON1,CON,Y,OVMR)                                  LAPC  10
C     ***** TRANSFORM CONIC TO PLOTTER HOMOGENEOUS COORDINATE SYSTEM ***LAPC  20
C     ***** CALLED BY SUBROUTINES LAP700 AND LAPAB *****                  LAPC  30
      DIMENSION CON1(7),CON(3,3),Y(3)                                     LAPC  40
      Y(1)=(CON1(1)+CON1(2))*0.5                                          LAPC  50
      Y(2)=(CON1(3)+CON1(4))*0.5                                          LAPC  60
      Y(3)=1.0                                                            LAPC  70
      CON(1,1)=CON1(5)                                                    LAPC  80
      CON(1,2)=CON1(6)                                                    LAPC  90
      CON(2,1)=CON1(6)                                                    LAPC 100
      CON(2,2)=CON1(7)                                                    LAPC 110
      T1=(CON1(2)-CON1(1)+CON1(4)-CON1(3))*0.25                           LAPC 120
      CON(3,3)=-((T1-OVMR)/T1)**2                                         LAPC 130
      DO 205 K=1,2                                                        LAPC 140
      CON(K,3)=0.0                                                        LAPC 150
      DO 200 J=1,2                                                        LAPC 160
  200 CON(K,3)=CON(K,3)-Y(J)*CON(J,K)                                     LAPC 170
      CON(3,K)=CON(K,3)                                                   LAPC 180
  205 CON(3,3)=CON(3,3)-CON(3,K)*Y(K)                                     LAPC 190
      RETURN                                                              LAPC 200
      END                                                                 LAPC 210


      SUBROUTINE LAPDRW(Y,NPEN,NCQ)                                       LAPD  10
C     ***** SUBROUTINE ELIMINATES HIDDEN LINES AND DRAWS VISIBLE LINES *LAPD  20
      DIMENSION CB(20),CQ(50,2),QL(4,30,2),SEG(2),Y(3),YN(3),YO(3),Z(3) LAPD  30
      COMMON/OLAP/CONIC(7,500),COVER(6,20),KC(20),KQ(30),NCONIC,NCOVER, LAPD  40
     1 NQOVER,NQUAD,OVMRGN,QOVER(3,4,30),QUAD(9,600),SEGM(50,2)          LAPD  50
      REAL*8 CHEM                                                         LAPD  60
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      LAPD  70
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) LAPD  80
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) LAPD  90
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) LAPD 100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   LAPD 110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   LAPD 120
      DIMENSION XLNG(3),XO(3),XT(3)                                     LAPD 130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   LAPD 140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,IATM,LTNO,NATOM,NCD LAPD 150
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1LAPD 160
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   LAPD 170
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                LAPD 180
      NCQ=NCOVER+NQOVER                                                 LAPD 190
      IF(NCQ)200,200,205                                                LAPD 200
  200 RETURN                                                            LAPD 210
C     ***** CHECK ALL OVERLAPPING ATOMS AND BONDS *****                 LAPD 220
  205 NPM3=NPEN-3                                                       LAPD 230
      IF(NPM3)  210,230,230                                             LAPD 240
C     ***** SAVE INFORMATION FROM LAST POINT IF PEN IS DOWN *****       LAPD 250
  210 YO(1)=YN(1)                                                       LAPD 260
      YO(2)=YN(2)                                                       LAPD 270
      YO(3)=1.0                                                         LAPD 280
      NPO=NPN                                                           LAPD 290
      DO 215 K=1,NCQ                                                    LAPD 300
  215 CQ(K,1)=CQ(K,2)                                                   LAPD 310
      IF(NQOVER)230,230,220                                             LAPD 320
  220 DO 225 K=1,NQOVER                                                 LAPD 330
      DO 225 J=1,4                                                      LAPD 340
  225 QL(J,K,1)=QL(J,K,2)                                               LAPD 350
C     ***** EVALUATE CONIC QUADRATIC FORMS AT NEW POINT YN *****        LAPD 360
  230 YN(1)=Y(1)                                                        LAPD 370
      YN(2)=Y(2)                                                        LAPD 380
      YN(3)=1.0                                                         LAPD 390
      NPN=NPEN                                                          LAPD 400
      IF(NCOVER)250,250,235                                             LAPD 410
  235 DO 245 K=1,NCOVER                                                 LAPD 420
      Z(1)=YN(1)*COVER(1,K)+YN(2)*COVER(2,K)+COVER(3,K)                 LAPD 430
      Z(2)=YN(1)*COVER(2,K)+YN(2)*COVER(4,K)+COVER(5,K)                 LAPD 440
      Z(3)=YN(1)*COVER(3,K)+YN(2)*COVER(5,K)+COVER(6,K)                 LAPD 450
      CQ(K,2)=Z(1)*YN(1)+Z(2)*YN(2)+Z(3)                                LAPD 460
C     ***** EVALUATE CONIC BILINEAR FORM IF PEN IS DOWN *****           LAPD 470
      IF(NPM3)240,245,245                                               LAPD 480
  240 CB(K)= Z(1)*YO(1)+Z(2)*YO(2)+Z(3)                                 LAPD 490
  245 CONTINUE                                                          LAPD 500
C     ***** EVALUATE LINEAR FORMS AND SIGNATURE FOR QUADRANGLE *****    LAPD 510
  250 IF(NQOVER)275,275,255                                             LAPD 520
  255 KCQ=NCOVER                                                        LAPD 530
      DO 270 K=1,NQOVER                                                 LAPD 540
      T2=3.0                                                            LAPD 550
      DO 265 J=1,4                                                      LAPD 560
      T1=YN(1)*QOVER(1,J,K)+YN(2)*QOVER(2,J,K)+QOVER(3,J,K)             LAPD 570
      IF(T1)260,265,265                                                 LAPD 580
  260 T2=T2-1.0                                                         LAPD 590
  265 QL(J,K,2)=T1                                                      LAPD 600
      KCQ=KCQ+1                                                         LAPD 610
C     ***** T2=-1 INSIDE, =0 ACROSS ANY EDGE, =1 ACROSS ANY VERTEX *****LAPD 620
  270 CQ(KCQ,2)=T2                                                      LAPD 630
C     ***** IF PEN IS UP, OMIT ALL SUBSEQUENT CHECKING *****            LAPD 640
  275 IF(NPM3)285,280,280                                               LAPD 650
  280 NPN=3                                                             LAPD 660
      CALL SCRIBE(YN,NPN,LTNC)                                          LAPD 670
      RETURN                                                            LAPD 680
C     ***** CHECK FOR HIDDEN SEGMENT *****                              LAPD 690
  285 DO 295 K=1,NCQ                                                    LAPD 700
      IF(CQ(K,1))290,295,295                                            LAPD 710
  290 IF(CQ(K,2))280,295,295                                            LAPD 720
  295 CONTINUE                                                          LAPD 730
C     ***** FIND ENTRY AND EXIT POINTS ON EACH CONIC *****              LAPD 740
      NINT=0                                                            LAPD 750
      IF(NCOVER)330,330,300                                             LAPD 760
  300 DO 325 K=1,NCOVER                                                 LAPD 770
C     ***** EVALUATE DISCRIMINANT *****                                 LAPD 780
      T1=CB(K)**2-CQ(K,1)*CQ(K,2)                                       LAPD 790
      IF(T1)325,325,305                                                 LAPD 800
  305 T1=SQRT(T1)                                                       LAPD 810
C     ***** SOLVE QUADRATIC EQATION *****                               LAPD 820
      T2=CQ(K,1)-CB(K)                                                  LAPD 830
      T3=T2+CQ(K,2)-CB(K)                                               LAPD 840
      IF(ABS(T3)-1.E-5)325,325,310                                      LAPD 850
  310 T4=(T2-T1)/T3                                                     LAPD 860
      T5=(T2+T1)/T3                                                     LAPD 870
C     ***** VALID INTERSECTION IF T4.LT.1 AND T5.GT.0 *****             LAPD 880
      IF(T4-1.0)315,325,325                                             LAPD 890
  315 IF(T5)325,325,320                                                 LAPD 900
C     ***** SAVE VALID CONIC INTERSECTIONS *****                        LAPD 910
  320 NINT=NINT+1                                                       LAPD 920
      SEGM(NINT,1)=T4                                                   LAPD 930
      SEGM(NINT,2)=T5                                                   LAPD 940
  325 CONTINUE                                                          LAPD 950
  330 IF(NQOVER)425,425,335                                             LAPD 960
C     ***** FIND ENTRY AND EXIT POINTS FOR EACH QUADRANGLE *****        LAPD 970
  335 DO 420 K=1,NQOVER                                                 LAPD 980
      I12=0                                                             LAPD 990
      KCQ=NCOVER+K                                                      LAPD1000
C     ***** CHECK FOR SINGLE INSIDE POINT *****                         LAPD1010
      SEG(1)=CQ(KCQ,1)                                                  LAPD1020
      IF(SEG(1))345,340,340                                             LAPD1030
  340 SEG(1)=1.0-CQ(KCQ,2)                                              LAPD1040
      IF(SEG(1)-1.0)350,350,345                                         LAPD1050
C     ***** INSIDE POINT FOUND, ONLY ONE INTERSECTION POSSIBLE *****    LAPD1060
  345 I12=1                                                             LAPD1070
C     ***** FIND WHICH EDGES ARE CROSSED BY THE SEGMENT *****           LAPD1080
  350 DO 410 J=1,4                                                      LAPD1090
      T1=QL(J,K,1)                                                      LAPD1100
      T2=QL(J,K,2)                                                      LAPD1110
      T3=T1-T2                                                          LAPD1120
      IF(T1*T2)355,355,410                                              LAPD1130
C     ***** CHECK FOR SEGMENT ON AN EDGE *****                          LAPD1140
  355 IF(ABS(T3)-1.E-5)420,420,360                                      LAPD1150
C     ***** CALCULATE COORDINATES OF INTERSECTION *****                 LAPD1160
  360 T4=(T1*YN(1)-T2*YO(1))/T3                                         LAPD1170
      T5=(T1*YN(2)-T2*YO(2))/T3                                         LAPD1180
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      J1=2*(MOD(J,4)+1)                                                 LAPD1190
      IQ=KQ(K)                                                          LAPD1200
C     ***** IS INTERSECTION WITHIN LIMITS OF QUADRANGLE *****           LAPD1210
      T6=(T4-QUAD(2*J-1,IQ))*(QUAD(J1-1,IQ)-T4)+(T5-QUAD(2*J,IQ))*      LAPD1220
     1 (QUAD(J1,IQ)-T5)                                                 LAPD1230
      IF(ABS(T6)-1.E-4)370,370,365                                      LAPD1240
  365 IF(T6)410,370,370                                                 LAPD1250
C     ***** CALCULATE FRACTION PARAMETER AND STORE IT *****             LAPD1260
  370 T1=T1/T3                                                          LAPD1270
      IF(I12-1)375,380,395                                              LAPD1280
C     ***** STORE FIRST INTERSECTION *****                              LAPD1290
  375 I12=1                                                             LAPD1300
      GO TO 390                                                         LAPD1310
C     ***** STORE SECOND INTERSECTION ****                              LAPD1320
  380 I12=2                                                             LAPD1330
      IF(T1-SEG(1))385,405,405                                          LAPD1340
  385 SEG(2)=SEG(1)                                                     LAPD1350
  390 SEG(1)= T1                                                        LAPD1360
      GO TO 410                                                         LAPD1370
C     ***** MORE THAN TWO INTERSECTIONS (I.E.,QUADRANGLE DIAGONAL) *****LAPD1380
  395 IF(T1-SEG(1))390,410,400                                          LAPD1390
  400 IF(T1-SEG(2))410,410,405                                          LAPD1400
  405 SEG(2)=T1                                                         LAPD1410
  410 CONTINUE                                                          LAPD1420
      IF(I12-1)420,420,415                                              LAPD1430
C     ***** STORE FRACTION PARAMETERS *****                             LAPD1440
  415 NINT=NINT+1                                                       LAPD1450
      SEGM(NINT,1)=SEG(1)                                               LAPD1460
      SEGM(NINT,2)=SEG(2)                                               LAPD1470
  420 CONTINUE                                                          LAPD1480
C     ***** END OF ENTRY-AND-EXIT-POINT CALCULATIONS *****              LAPD1490
  425 IF(NINT-1)430,490,435                                             LAPD1500
C     ***** NO INTERFERENCE FOUND, DRAW ENTIRE SEGMENT *****            LAPD1510
  430 CALL SCRIBE(YN,2,LTNO)                                            LAPD1520
      RETURN                                                            LAPD1530
C     **** SORT SEGMENT INTERSECTION LIST *****                         LAPD1540
C     ***** SORTING PROCEDURE BY SHELL,D.L. COMM. ACM 2,30-32 (1959) ***LAPD1550
  435 M=NINT                                                            LAPD1560
  440 M=M/2                                                             LAPD1570
      IF(M)490,490,445                                                  LAPD1580
  445 K=NINT-M                                                          LAPD1590
      J=1                                                               LAPD1600
  450 I=J                                                               LAPD1610
  455 IM=I+M                                                            LAPD1620
      IF(SEGM(I,1))460,470,470                                          LAPD1630
  460 IF(SEGM(IM,1))465,465,485                                         LAPD1640
  465 IF(SEGM(I,2)-SEGM(IM,2))485,485,475                               LAPD1650
  470 IF(SEGM(I,1)-SEGM(IM,1))485,485,475                               LAPD1660
  475 DO 480 L=1,2                                                      LAPD1670
      T1=SEGM(I,L)                                                      LAPD1680
      SEGM(I,L)=SEGM(IM,L)                                              LAPD1690
  480 SEGM(IM,L)=T1                                                     LAPD1700
      I=I-M                                                             LAPD1710
      IF(I)485,485,455                                                  LAPD1720
  485 J=J+1                                                             LAPD1730
      IF(J-K)450,450,440                                                LAPD1740
C     ***** FIND STARTING POINT P0 AND END POINT P1 *****               LAPD1750
  490 P0=0.0                                                            LAPD1760
      K=0                                                               LAPD1770
  495 K=K+1                                                             LAPD1780
      IF(K-NINT)500,500,515                                             LAPD1790
  500 P1=SEGM(K,1)                                                      LAPD1800
      IF(P1)510,505,505                                                 LAPD1810
  505 IF(P1-P0)510,510,520                                              LAPD1820
  510 P0=AMAX1(P0,SEGM(K,2))                                            LAPD1830
      IF(P0-1.0)495,530,525                                             LAPD1840
  515 P1=1.0                                                            LAPD1850
C     ***** DRAW SEGMENT FROM P0 TO P1 *****                            LAPD1860
  520 IF(P0)535,535,530                                                 LAPD1870
  525 P0=1.0                                                            LAPD1880
  530 Z(1)=YO(1)*(1.-P0)+YN(1)*P0                                       LAPD1890
      Z(2)=YO(2)*(1.-P0)+YN(2)*P0                                       LAPD1900
      NPN=3                                                             LAPD1910
      CALL SCRIBE(Z,NPN,LTNO)                                           LAPD1920
      IF(P0-1.0)535,540,540                                             LAPD1930
  535 Z(1)=YO(1)*(1.-P1)+YN(1)*P1                                       LAPD1940
      Z(2)=YO(2)*(1.-P1)+YN(2)*P1                                       LAPD1950
      NPN=2                                                             LAPD1960
      CALL SCRIBE(Z,NPN,LTNO)                                           LAPD1970
      IF(P1-1.0)510,540,540                                             LAPD1980
  540 RETURN                                                            LAPD1990
      END                                                               LAPD2000
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      SUBROUTINE MM(X,Y,Z)                                              MM     10
C     MULTIPLY TWO MATRICES                                             MM     20
C     Z(3,3)=X(3,3)*Y(3,3)                                              MM     30
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                    MM     40
      DO 117 I=1,3                                                      MM     50
      DO 117 K=1,3                                                      MM     60
      Z(I,K)=0.0                                                        MM     70
      DO 117 J=1,3                                                      MM     80
  117 Z(I,K)=Z(I,K)+X(I,J)*Y(J,K)                                       MM     90
      RETURN                                                            MM    100
      END                                                               MM    110


      SUBROUTINE MV(X,Y,Z)                                              MV     10
C     MATRIX * VECTOR                                                   MV     20
C     Z(3)=X(3,3)*Y(3)                                                  MV     30
      DIMENSION X(3,3),Y(3),Z(3)                                        MV     40
      DO 113 I=1,3                                                      MV     50
      Z(I)=0.0                                                          MV     60
      DO 113 J=1,3                                                      MV     70
  113 Z(I)=Z(I)+X(I,J)*Y(J)                                             MV     80
      RETURN                                                            MV     90
      END                                                               MV    100


      SUBROUTINE NORM(X,Y,Z,ITYPE)                                      NORM   10
C     ***** VECTOR PRODUCT  Z=X*Y *****                                 NORM   20
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         NORM   30
      DIMENSION X(3),Y(3),Z(3),Z1(3)                                    NORM   40
      REAL*8 CHEM                                                       NORM   50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    NORM   60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)NORM   70
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) NORM   80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) NORM   90
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   NORM  100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   NORM  110
      DIMENSION XLNG(3),XO(3),XT(3)                                     NORM  120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   NORM  130
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD NORM  140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1NORM  150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   NORM  160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                NORM  170
      DO 125 J=1,3                                                      NORM  180
      I1=MOD(I+3,3)+1                                                   NORM  190
      I2=MOD(I+1,3)+1                                                   NORM  200
      T1=X(I1)*Y(I2)-X(I2)*Y(I1)                                        NORM  210
      IF(ITYPE)115,115,105                                              NORM  220
  105 Z(I)=T1                                                           NORM  230
      GO TO 125                                                         NORM  240
  115 Z1(I)=T1                                                          NORM  250
  125 CONTINUE                                                          NORM  260
      IF(ITYPE)135,135,300                                              NORM  270
  135 CALL MV(BB,Z1,Z)                                                  NORM  280
  300 RETURN                                                            NORM  290
      END                                                               NORM  300


      SUBROUTINE PAXES(ACODE,ITYPE)                                     PAXE   10
C     ***** ITYPE .LT.0 FOR COVARIANCE MATRIX IN Q *****                PAXE   20
C     ***** ITYPE .GT.0 FOR ELLIPSOID QUADRATIC FORM IN Q *****         PAXE   30
C     ***** XABSF(ITYPE)=1 BASED ON TRICLINIC COORDINATE SYSTEM *****   PAXE   40
C     ***** =2 OR 3 FOR WORKING OR REFERENCE CARTESIAN SYSTEMS *****    PAXE   50
C     ***** CONTRAVARIANT EIGENVECTORS FOR Q IN COLUMNS OF PAC *****    PAXE   60
C     ***** CHECK ATOM CODE *****                                       PAXE   70
      DIMENSION W(3,3),X(3)                                             PAXE   80
      REAL*8 CHEM                                                       PAXE   90
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PAXE  100
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)PAXE  110
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PAXE  120
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PAXE  130
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PAXE  140
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PAXE  150
      DIMENSION XLNG(3),XO(3),XT(3)                                     PAXE  160
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PAXE  170
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PAXE  180
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PAXE  190
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PAXE  200
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PAXE  210
      IT=IABS(ITYPE)-1                                                  PAXE  220
      KS=AMOD(ACODE,100.)                                               PAXE  230
      IF(NSYM-KS)105,115,115                                            PAXE  240
  105 NG=4                                                              PAXE  250
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      GO TO 300                                                         PAXE 260
  115 II=ACODE/100000.                                                  PAXE 270
      IF(NATOM-II) 125,130,130                                          PAXE 280
  125 NG=5                                                              PAXE 290
      GO TO 300                                                         PAXE 300
  130 IF(II) 125,125,135                                                PAXE 310
C     ***** CRYSTALLOGRAPHIC SYMMETRY ROTATION *****                    PAXE 320
  135 CALL TMM(PA(1,1,II),PS(1,1,KS),PAT)                               PAXE 330
      IF(IT-1) 160,145,155                                              PAXE 340
C     ***** TRANSFORM TO CARTESIAN SYSTEMS *****                        PAXE 350
  145 CALL TMM(PAT,AAWRK,PAC)                                           PAXE 360
      GO TO 175                                                         PAXE 370
  155 CALL TMM(PAT,AAREV,PAC)                                           PAXE 380
      GO TO 175                                                         PAXE 390
  160 IF(ITYPE) 162,155,170                                             PAXE 400
C     ***** TRANSFORM TO TRICLINIC SYSTEM *****                         PAXE 410
  162 DO 165 J=1,9                                                      PAXE 420
  165 PAC(J,1)=PAT(J,1)                                                 PAXE 430
      GO TO 175                                                         PAXE 440
  170 CALL MM(AA,PAT,PAC)                                               PAXE 450
C     ***** FORM DIAGONAL MATRIX OR ITS INVERSE *****                   PAXE 460
  175 DO 205 J=1,3                                                      PAXE 470
      T1=EV(J,II)                                                       PAXE 480
      IF(ITYPE) 195,195,185                                             PAXE 490
  185 X(J)=1./(T1*T1)                                                   PAXE 500
      GO TO 205                                                         PAXE 510
  195 X(J)=T1*T1                                                        PAXE 520
  205 RMS(J)=T1                                                         PAXE 530
C     ***** FORM QUADRATIC FORM *****                                   PAXE 540
      DO 245 I=1,3                                                      PAXE 550
      DO 245 J=I,3                                                      PAXE 560
      T1=0.0                                                            PAXE 570
      DO 225 K=1,3                                                      PAXE 580
  225 T1=T1+PAC(I,K)*PAC(J,K)*X(K)                                      PAXE 590
      Q(J,I)=T1                                                         PAXE 600
  245 Q(I,J)=T1                                                         PAXE 610
  300 RETURN                                                            PAXE 620
      END                                                               PAXE 630


      SUBROUTINE PLTXY(X,Y)                                             PLTX  10
C     ***** PLCT COORD. AND CLOSEST EDGE AFTER PROJECTION *****         PLTX  20
      DIMENSION X(3),Y(2)                                               PLTX  30
      REAL*8 CHEM                                                       PLTX  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PLTX  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) PLTX  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PLTX  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PLTX  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PLTX  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PLTX 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     PLTX 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PLTX 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PLTX 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PLTX 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PLTX 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PLTX 160
      T4=1.                                                             PLTX 170
      T1=1.                                                             PLTX 180
      IF(VIEW) 125,125,110                                              PLTX 190
  110 T4=VIEW-X(3)                                                      PLTX 200
      IF(T4) 115,115,120                                                PLTX 210
  115 Y(1)=-99.                                                         PLTX 220
      Y(2)=-99.                                                         PLTX 230
      GO TO 130                                                         PLTX 240
  120 T1=VIEW/T4                                                        PLTX 250
  125 Y(1)=X(1)*T1+XO(1)                                                PLTX 260
      Y(2)=X(2)*T1+XO(2)                                                PLTX 270
      T1=XLNG(1)-ABS(Y(1)*2.-XLNG(1))                                   PLTX 280
      T2=XLNG(2)-ABS(Y(2)*2.-XLNG(2))                                   PLTX 290
      EDGE=AMIN1(T1,T2)*.5                                              PLTX 300
      IF(T4-VIEW*.5) 130,300,300                                        PLTX 310
  130 EDGE=-99.                                                         PLTX 320
  300 RETURN                                                            PLTX 330
      END                                                               PLTX 340


      SUBROUTINE PRELIM                                                 PREL  10
C     ***** DATA INPUT ROUTINE *****                                    PREL  20
      DIMENSION B(9)                                                    PREL  30
      REAL*8 CHEM                                                       PREL  40
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PREL  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) PREL  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PREL  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PREL  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PREL  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PREL 100
      DIMENSION XLNG(3),XO(3),XT(3)                                     PREL 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PREL 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PREL 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PREL 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PREL 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PREL 160
C     ***** CELL DIMENSIONS *****                                       PREL 170
  106 FORMAT(6F9.6)                                                     PREL 180
      READ (IN,106) (A(I),I=1,6)                                        PREL 190
      T1=ABS(A(4))-1.                                                   PREL 200
      DO 125 J=1,3                                                      PREL 210
      IF(T1) 115,110,110                                                PREL 220
C     ***** CELL ANGLES IN DEGREES *****                                PREL 230
  110 A(J+6)=A(J+3)                                                     PREL 240
      A(J+3)=COS(A(J+6)*1.745329E-2)                                    PREL 250
      GO TO 120                                                         PREL 260
C     ***** COSINES OF CELL ANGLES *****                                PREL 270
  115 A(J+6)=ARCCOS(A(J+3))                                             PREL 280
C     ***** STORE IDEMFACTOR MATRIX *****                               PREL 290
  120 AID(J,J)=1.                                                       PREL 300
      AID(J+1,1)=0.                                                     PREL 310
      AID(J+5,1)=0.                                                     PREL 320
C     ***** STORE METRIC TENSOR *****                                   PREL 330
  125 AA(J,J)=A(J)**2                                                   PREL 340
      AA(1,2)=A(1)*A(2)*A(6)                                            PREL 350
      AA(1,3)=A(1)*A(3)*A(5)                                            PREL 360
      AA(2,3)=A(2)*A(3)*A(4)                                            PREL 370
      AA(2,1)=AA(1,2)                                                   PREL 380
      AA(3,1)=AA(1,3)                                                   PREL 390
      AA(3,2)=AA(2,3)                                                   PREL 400
C     ***** INVERT METRIC TENSOR *****                                  PREL 410
      CALL AXEQB(AA,BB,AID,3)                                           PREL 420
C     ***** CALCULATE RECIPROCAL CELL PARAMETERS *****                  PREL 430
      DO 128 J=1,3                                                      PREL 440
  128 B(J)=SQRT(BB(J,J))                                                PREL 450
      B(6)=BB(1,2)/(B(1)*B(2))                                          PREL 460
      B(5)=BB(1,3)/(B(1)*B(3))                                          PREL 470
      B(4)=BB(2,3)/(B(2)*B(3))                                          PREL 480
      DO 130 J=1,3                                                      PREL 490
  130 B(J+6)=ARCCOS(B(J+3))                                             PREL 500
C     ***** WAS INPUT FOR REAL OR RECIPROCAL CELL *****                 PREL 510
      IF(A(1)-1.) 135,150,150                                           PREL 520
  135 DO 140 J=1,9                                                      PREL 530
      T1=AA(J,1)                                                        PREL 540
      AA(J,1)=BB(J,1)                                                   PREL 550
      BB(J,1)=T1                                                        PREL 560
      T1=A(J)                                                           PREL 570
      A(J)=B(J)                                                         PREL 580
  140 B(J)=T1                                                           PREL 590
C     ***** WRITE OUT CELL PARAMETERS *****                             PREL 600
  143 FORMAT(1H010X,22HDIRECT CELL PARAMETERS/1H 15X,1HA14X,1HB14X,1HC14PREL 610
     1X,5HALPHA10X,4HBETA11X,5HGAMMA)                                   PREL 620
  145 FORMAT(1H 10X,F9.6,2F15.6,3F15.3/1H 48X,6HCOSINEF12.8,2F15.8)     PREL 630
  147 FORMAT(1H010X,26HRECIPROCAL CELL PARAMETERS/1H 15X,2HA*13X,2HB*13XPREL 640
     1,2HC*13X,6HALPHA*9X,5HBETA*10X,6HGAMMA*)                          PREL 650
  150 WRITE (NOUT,143)                                                  PREL 660
      WRITE (NOUT,145) (A(I),I=1,3),(A(I),I=7,9),(A(I),I=4,6)           PREL 670
      WRITE (NOUT,147)                                                  PREL 680
      WRITE (NOUT,145) (B(I),I=1,3),(B(I),I=7,9),(B(I),I=4,6)           PREL 690
C     ***** STORE STANDARD VECTORS *****                                PREL 700
      CALL AXES(AID,AID(1,2),REFV,0)                                    PREL 710
      CALL MM(AA,REFV,AAREV)                                            PREL 720
      DO 160 I=1,3                                                      PREL 730
      DO 160 J=1,3                                                      PREL 740
      AAWRK(J,I)=AAREV(J,I)                                             PREL 750
      Q(J,I)=REFV(I,J)                                                  PREL 760
  160 WRKV(J,I)=REFV(J,I)                                               PREL 770
C     ***** READ AND WRITE SYMMETRY TRANSFORMATIONS *****               PREL 780
  171 FORMAT(1H010X,24HSYMMETRY TRANSFORMATIONS/1H 14X,3HNO.12X,13HTRANSPREL 790
     1FORMED X18X,13HTRANSFORMED Y18X,13HTRANSFORMED Z)                 PREL 800
  173 FORMAT(I1,F14.10,3F3.0,2(F15.10,3F3.0))                           PREL 810
  175 FORMAT(1H 13X,I2,3(F13.6,F4.0,2H XF4.0,2H YF4.0,2H Z))            PREL 820
  177 FORMAT(1H110X,18A4)                                               PREL 830
      WRITE (NOUT,171)                                                  PREL 840
      LINES=14                                                          PREL 850
      DO 190 I=1,48                                                     PREL 860
      LINES=MOD(LINES+1,56)                                             PREL 870
      READ (IN,173) IS,(TS(J,I),(FS(K,J,I),K=1,3),J=1,3)                PREL 880
      IF(LINES) 185,180,185                                             PREL 890
  180 WRITE (NOUT,177) (TITLE(J),J=1,18)                                PREL 900
      WRITE (NOUT,171)                                                  PREL 910
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  185 WRITE (NOUT,175)I,(TS(J,I),(PS(K,J,I),K=1,3),J=1,3)
C     ***** NON-CRYSTALLOGRAPHIC HELIX-SYMMETRY INPUT *****
      IF(PS(3,3,I)-5.)188,186,186
  186 T1=PS(1,3,I)/PS(3,3,I)
      TS(3,I)=TS(3,I)+T1
      T1=AMOD(T1*PS(2,3,I),1.)*6.28318531
      T2=COS(T1)
      T1=SIN(T1)
      DO 187 J=1,9
  187 VT(J,1)=AID(J,1)
      VT(1,1)=T2
      VT(2,2)=T2
      VT(2,1)=-T1
      VT(1,2)=T1
      CALL MM(VT,Q,PAC)
      CALL MM(AAREV,PAC,PS(1,1,I))
  188 IF(IS)195,190,195
  190 CONTINUE
      NG=1
      CALL ERPNT(0.,0)
      I=48
  195 NSYM=I
C     ***** POSITIONAL AND THERMAL PARAMETERS *****
  207 FORMAT(11HO NO. ATOM 8X,1HX10X,1HY10X,1HZ13X,3HB118X,3HB228X,3HB33
     18X,3HB128X,3HB138X,10HB23    TYPE)
  209 FORMAT(1H I3,1X,A6,3F11.6,5X,6F11.6,F5.0)
  210 FORMAT(1H I3,1X,A6,3F11.6,5X,2F11.6,4F11.0,F5.0)
  211 FORMAT(A6,3X,5F9.6,F9.0)
  213 FORMAT(I1,F8.6,5F9.6,7X,F2.0)
      LINES=LINES+2
      IF(LINES-56)220,215,215
  215 LINES=-1
      GO TO 225
  220 WRITE (NOUT,207)
  225 DO 245 I=1,166
      LINES=MOD(LINES+1,56)
      READ (IN,211)CHEM(I),V1(1),V1(2),(P(J,I),J=1,3),T1
      K=1.+T1
      IF(FLOAT(K-1)-T1)227,228,227
  227 K=1
  228 READ (IN,213)IS,(PA(J,1,I),J=1,7)
      IF(LINES)230,230,232
  230 WRITE (NOUT,177)(TITLE(J),J=1,18)
      WRITE (NOUT,207)
  232 IF(PA(3,1,I)-10000.)235,234,234
  234 WRITE (NOUT,210)I,CHEM(I),(P(J,I),J=1,3),(PA(J,1,I),J=1
     1,7)
      GO TO 238
  235 WRITE (NOUT,209)I,CHEM(I),(P(J,I),J=1,3),(PA(J,1,I),J=1
     1,7)
  238 GO TO (244,239,241,242,244),K
C     ***** TYPE 1 POSITIONAL PARAMETERS (ANGSTROMS) *****
  239 DO 240 J=1,3
  240 P(J,I)=P(J,I)/A(J)
      GO TO 244
C     ***** TYPE 2 POSITIONAL PARAMETERS, STANDARD CARTESIAN *****
  241 V1(1)=P(1,I)
      V1(2)=P(2,I)
      GO TO 243
C     ***** TYPE 3 POSITIONAL PARAMETERS *****
C     ***** CYLINDRICAL COORDINATES REFERRED TO STANDARD CARTESIAN *****
  242 T2=P(2,I)*.01745329252
      V1(1)=V1(1)+P(1,I)*COS(T2)
      V1(2)=V1(2)+P(1,I)*SIN(T2)
  243 V1(3)=P(3,I)
      CALL VM(V1,Q,P(1,I))
  244 IF(IS)246,245,246
  245 CONTINUE
      NG=2
      CALL ERPNT(0.,0)
      I=100
  246 NATOM=I
C     ***** CONVERT TEMP FACTOR COEF TO STANDARD TYPE ZERO *****
      NG1=0
      DO 450 I=1,NATOM
      T1=PA(1,1,I)
      K=1.+PA(7,1,I)
      IF(T1)250,250,255
  250 T1=.1
      GO TO 405
  255 T6=.0506605918
      GO TO(270,260,265,265,270,260,400,405,270,260,270,450),K
C     ***** TYPE 1 *****
  260 DO 262 J=4,6
  262 PA(J,1,I)=PA(J,1,I)*.5
      GO TO 270
C     ***** TYPES 2 AND 3 (BASE 2 SYSTEMS) *****
  265 T6=.351152464
      IF(K-4)270,260,270
C     ***** TYPES 0 THROUGH 5 *****
  270 IF(PA(2,1,I))400,400,272
  272 DO 300 J=1,3
      DO 300 L=J,3
      T2=T6
      IF(K-5)285,275,275
  275 IF(K-6)280,280,281
C     ***** TYPES 4 AND 5 *****
  280 T2=B(J)*B(L)*T2*.25
      GO TO 285
C     ***** TYPES 8 AND 9 (U(I,J) TENSOR SYSTEMS) *****
  281 T2=B(J)*B(L)
      IF(K-11)285,282,282
C     ***** TYPE 10, (CARTESIAN TENSOR SYSTEM) *****
  282 T2=1.0
  285 IF(J-L)290,287,290
  287 VT(J,J)=T2*PA(J,1,I)
      GO TO 300
  290 M=J+L+1
      VT(J,L)=T2*PA(M,1,I)
      VT(L,J)=VT(J,L)
  300 CONTINUE
C     ***** FIND PRINCIPAL AXES *****
      IF(K-11)310,305,305
  305 CALL MM(VT,Q,PAC)
      CALL MM(REFV,PAC,VT)
  310 CALL MM(VT,AA,DA)
      CALL EIGEN(DA,RMS,PAT)
C     ***** ARE EIGENVALUES POSITIVE *****
      IF(RMS(1))325,325,320
  320 IF(NG)350,360,330
  325 NG=3
  330 NG1=1
      CALL ERPNT(FLOAT(I)*100000.+55501.,0)
C     ***** 3 EQUAL EIGENVALUES, USE REFERENCE VECTORS *****
  340 T3=SIGN(SQRT(ABS(RMS(1)+RMS(2)+RMS(3))/3.),RMS(1))
      DO 345 J=1,3
      DO 342 K=1,3
  342 PA(J,K,I)=REFV(J,K)
  345 EV(J,I)=T3
      GO TO 450
  350 IF(NG+6)340,340,352
C     ***** TWO EQUAL EIGENVALUES *****
  352 N=NG+5
      CALL UNIT(PAT(1,N),V1,-1)
      DO 354 K=1,3
      IF(ABS(VMV(V1,AA,REFV(1,K)))-.58)356,354,354
  354 CONTINUE
  356 CALL MM(AA,DA,VT)
      CALL AXES(V1,REFV(1,K),DA,-1)
      DO 359 K=1,3
      L=MOD(N+K-2,3)+1
      DO 358 J=1,3
  358 PA(J,L,I)=DA(J,K)
  359 EV(L,I)=SIGN(SQRT(ABS(VMV(DA(1,K),VT,DA(1,K)))),RMS(L))
      GO TO 450
C     ***** MAKE EIGENVECTORS 1 ANGSTROM LONG *****
  360 CALL AXES(PAT(1,1),PAT(1,3),PA(1,1,I),-1)
  370 NG=0
C     ***** SQRT EIGENVALUE = RMS DISPLACEMENT *****
      DO 375 J=1,3
      T2=RMS(J)
  375 EV(J,I)=SIGN(SQRT(ABS(T2)),T2)
      GO TO 450
C     ***** TYPE 6 (ISOTROPIC TEMP FACTOR) *****
  400 T1=SQRT(T1*1.266515E-2)
C     ***** TYPE 7 (DUMMY SPHERE) *****
  405 DO 410 J=1,3
  410 EV(J,I)=T1
      IF(PA(3,1,I))430,430,415
C     ***** DEFINED VECTORS FOR SPHERE *****
  415 DO 425 J=1,4
      T2=PA(J+2,1,I)
      CALL ATOM(T2,VT(1,J))
      IF(NG)420,425,420
  420 CALL ERPNT(T2,0)
      GO TO 430
  425 CONTINUE
      CALL DIFV(VT(1,2),VT(1,1),V1)
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      CALL DIFV(VT(1,4),VT(1,3),V2)                                     PREL2600
      CALL AXES(V1,V2,PA(1,1,I),-1)                                     PREL2610
      GO TO 450                                                         PREL2620
C     ***** REFERENCE VECTORS FOR SPHERE *****                          PREL2630
  430 DO 435 J=1,9                                                      PREL2640
  435 PA(J,1,I)=REFV(J,1)                                               PREL2650
  450 NG=0                                                              PREL2660
C     ***** WRITE OUT RMS VALUES *****                                  PREL2670
      LINES=LINES+2                                                     PREL2680
      IF(LINES-56)458,458,455                                           PREL2690
  455 LINES=-1                                                          PREL2700
      GO TO 460                                                         PREL2710
  458 WRITE (NOUT,461)                                                  PREL2720
  460 DO 465 I=1,NATOM                                                  PREL2730
      LINES=MOD(LINES+1,56)                                             PREL2740
      IF(LINES)465,462,465                                              PREL2750
  461 FORMAT(10HONO. ATOM 8X,1HX10X,1HY10X,1HZ13X,7HRMSD 1 4X,7HRMSD 2 4PREL2760
     1X,7HRMSD 3 )                                                      PREL2770
  462 WRITE (NOUT,177) (TITLE(J),J=1,18)                                PREL2780
      WRITE (NOUT,461)                                                  PREL2790
  463 FORMAT(1H I3,1X,A6,3F11.6)                                        PREL2800
  465 WRITE (NOUT,209)I,CHEM(I),(P(J,I),J=1,3),(EV(J,I),J=1,3           PREL2810
     1)                                                                 PREL2820
      IF(NG1)999,999,470                                                PREL2830
  470 CALL EXIT                                                         PREL2840
  999 RETURN                                                            PREL2850
      END                                                               PREL2860


      SUBROUTINE PRIME                                                  PRIM  10
C     ****GENERAL INITIALIZATION OF PRIME PARAMETERS****                PRIM  20
      REAL*8 CHEM                                                       PRIM  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PRIM  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)PRIM  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) PRIM  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PRIM  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   PRIM  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PRIM  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     PRIM 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PRIM 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD PRIM 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1PRIM 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PRIM 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PRIM 150
      BRDR=0.5                                                          PRIM 160
C     ****CALCULATE CONSTANTS****                                       PRIM 170
      DO 2999 I=1,5                                                     PRIM 180
 2999 CONT(I)=SQRT(1./(2.*(1.+COS(3.141593   /2.**I))))                 PRIM 190
      DISP=.005                                                         PRIM 200
      FORE=.866                                                         PRIM 210
      IN=5                                                              PRIM 220
      ITILT=0                                                           PRIM 230
      LATM=0                                                            PRIM 240
      NCD=0                                                             PRIM 250
      NG=0                                                              PRIM 260
      NOUT=6                                                            PRIM 270
      NSR=8                                                             PRIM 280
      RES(1)=1.25                                                       PRIM 290
      RES(2)=.5                                                         PRIM 300
      RES(3)=.2                                                         PRIM 310
      SCAL1=1.0                                                         PRIM 320
      SCAL2=1.54                                                        PRIM 330
      SCL=1.54                                                          PRIM 340
      DO 3000 I=1,3                                                     PRIM 350
      SYMB(I,I)=1.                                                      PRIM 360
      SYMB(I+1,1)=0.                                                    PRIM 370
 3000 SYMB(I+5,1)=0.                                                    PRIM 380
      TAPER=.375                                                        PRIM 390
      THETA=0.0                                                         PRIM 400
      VIEW=0.0                                                          PRIM 410
      XLNG(1)=17.0                                                      PRIM 420
      XLNG(2)=11.0                                                      PRIM 430
      XO(1)=8.5                                                         PRIM 440
      XO(2)=5.5                                                         PRIM 450
      DO 3001 J=1,3                                                     PRIM 460
 3001 ORGN(J) = 0.0                                                     PRIM 470
C     ***** INITIATE OVERLAP ROUTINES *****                             PRIM 480
      CALL LAP500(0)                                                    PRIM 490
      RETURN                                                            PRIM 500
      END                                                               PRIM 510


      SUBROUTINE PROJ(D,DP,X,XO,VIEW,I1,I2,I3)                          PROJ  10
C     ***** 3D CARTESIAN TO 2D PLOTTER COORDINATES *****                PROJ  20
      DIMENSION D(3,129),DP(2,129),X(3),XO(3)                           PROJ  30
      T3=VIEW-X(3)                                                      PROJ  40
      DO 145 I=I1,I2,I3                                                 PROJ  50
      T1=D(1,I)+X(1)                                                    PROJ  60
      T2=D(2,I)+X(2)                                                    PROJ  70
      IF(VIEW) 135,135,120                                              PROJ  80
  120 T4=VIEW/(T3-D(3,I))                                               PROJ  90
      T1=T1*T4                                                          PROJ 100
      T2=T2*T4                                                          PROJ 110
  135 DP(1,I)=T1+XO(1)                                                  PROJ 120
  145 DP(2,I)=T2+XO(2)                                                  PROJ 130
      RETURN                                                            PROJ 140
      END                                                               PROJ 150


      SUBROUTINE RADIAL(ND)                                             RADI  10
C     ***** GENERATE ELLIPSE FROM TWO CONJUGATE VECTORS *****           RADI  20
C     ***** ORTHONORMAL VECTORS PRODUCE 8-128 SPOKED CIRCLE *****       RADI  30
C     ***** ND DENOTES NUMBER OF SUBDIVISIONS (1 TO 5) *****            RADI  40
      REAL*8 CHEM                                                       RADI  50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    RADI  60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)RADI  70
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) RADI  80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) RADI  90
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   RADI 100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   RADI 110
      DIMENSION XLNG(3),XO(3),XT(3)                                     RADI 120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   RADI 130
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD RADI 140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1RADI 150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   RADI 160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                RADI 170
      DO 115 J=1,3                                                      RADI 180
      T1=DA(J,1)                                                        RADI 190
      D(J,1)=T1                                                         RADI 200
      D(J,129)=T1                                                       RADI 210
      D(J,65)=-T1                                                       RADI 220
      T1=DA(J,2)                                                        RADI 230
      D(J,33)=T1                                                        RADI 240
  115 D(J,97)=-T1                                                       RADI 250
      DO 135 K=1,ND                                                     RADI 260
      T1=CONT(K)                                                        RADI 270
      KDEL=2**(6-K)                                                     RADI 280
      KDEL1=KDEL+1                                                      RADI 290
      KDEL2=KDEL/2                                                      RADI 300
      DO 135 L=KDEL1,65,KDEL                                            RADI 310
      J=L-KDEL                                                          RADI 320
      M=L-KDEL2                                                         RADI 330
      DO 135 N=1,3                                                      RADI 340
      T2=(D(N,L)+D(N,J))*T1                                             RADI 350
      D(N,M)=T2                                                         RADI 360
  135 D(N,M+64)=-T2                                                     RADI 370
      RETURN                                                            RADI 380
      END                                                               RADI 390


      SUBROUTINE SCRIBE(Y,NPEN,LTNO)                                    SCRI  10
      DIMENSION Y(2),YO(2)                                              SCRI  20
C     ***** SUBROUTINE WHICH LINKS WITH THE PLOTTER-SPECIFIC SUBROUTINESSCRI  30
      IF(NPEN-3) 210,205,205                                            SCRI  40
C     ***** KEEP TRACK OF COORDINATES FOR LAST PEN-UP LOCATION *****    SCRI  50
  205 YO(1)=Y(1)                                                        SCRI  60
      YO(2)=Y(2)                                                        SCRI  70
      NPO=0                                                             SCRI  80
      RETURN                                                            SCRI  90
  210 IF(LTNO) 230,245,215                                              SCRI 100
C     ***** CALL MECHANICAL PLOTTER PLOTTING SUBROUTINE *****           SCRI 110
  215 IF(NPO) 225,220,225                                               SCRI 120
  220 CALL PLOT(YO(1),YO(2),3)                                          SCRI 130
  225 CALL PLOT(Y(1),Y(2),2)                                            SCRI 140
      GO TO 245                                                         SCRI 150
C     ***** CALL CRT PLOTTING SUBROUTINE *****                          SCRI 160
  230 IF(NPO) 240,235,240                                               SCRI 170
  235 CALL CRT(YO(1),YO(2),0,1)                                         SCRI 180
  240 CALL CRT(Y(1),Y(2),-LTNO,1)                                       SCRI 190
  245 NPO=1                                                             SCRI 200
      RETURN                                                            SCRI 210
      END                                                               SCRI 220


      SUBROUTINE SEARC                                                  SEAR  10
      DIMENSION NW(6),DX(3),S(2,200),U(3),V(3),W(2,4),WW(2,3),X(4),Y(3) SEAR  20
      DIMENSION Z(3)                                                    SEAR  30
      REAL*8 CHEM                                                       SEAR  40
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      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)     SEAR  50
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130) SEAR  60
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)  SEAR  70
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)  SEAR  80
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)    SEAR  90
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)    SEAR 100
      DIMENSION XLNG(3),XO(3),XT(3)                                      SEAR 110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D    SEAR 120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD  SEAR 130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1SEAR 140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2    SEAR 150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                 SEAR 160
C     ***** OBTAIN PROBLEM PARAMETERS *****                              SEAR 170
      WRITE (NOUT,20)                                                    SEAR 180
   20 FORMAT(1H0 9X,82H          FROM ATOMS    TO ATOMS     WITH RADIUS ORSEAR 190
     1, IF A BOX, WITH SEMIDIMENSIONS  /11X,46HCODE    (MIN  MAX)    (MIN SEAR 200
     2 MAX)                  7X,1HA8X,1HB8X,1HC)                        SEAR 210
      IF(AIN(1)-10000.)100,100,101                                       SEAR 220
  100 ITOM1=AIN(1)                                                       SEAR 230
      SYITOM=55501.                                                      SEAR 240
      GO TO 103                                                          SEAR 250
  101 ITOM1=AIN(1)/100000.                                               SEAR 260
      SYITOM=AMOD(AIN(1),100000.)                                        SEAR 270
  102 IF(ABS(AIN(2))-10000.) 103,103,104                                 SEAR 280
  103 ITOM2 = ABS(AIN(2))                                                SEAR 290
      SYITO2=SYITOM                                                      SEAR 300
      GO TO 105                                                          SEAR 310
  104 ITOM2=ABS(AIN(2))/100000.                                          SEAR 320
      SYITO2=AMOD(ABS(AIN(2)),100000.)                                   SEAR 330
  105 ITAR1=AIN(3)                                                       SEAR 340
      IF(ITAR1) 108,108,110                                              SEAR 350
  108 ITAR1=1                                                            SEAR 360
  110 ITAR2=AIN(4)                                                       SEAR 370
      DMAX=AIN(5)                                                        SEAR 380
      IF(DMAX) 115,115,120                                               SEAR 390
  115 DMAX=4.                                                            SEAR 400
      AIN(5)=DMAX                                                        SEAR 410
  120 DMX=DMAX*DMAX                                                      SEAR 420
      TEM=.01                                                            SEAR 430
      KFUN=NJ*100+MOD(NJ2,10)                                            SEAR 440
      K=NJ*100+NJ2                                                       SEAR 450
      IO=SYITOM                                                          SEAR 460
      IO2=SYITO2                                                         SEAR 470
      LATOM=LATM                                                         SEAR 480
  121 FORMAT(1H010X,2I3,I5,I4,I5,2I4,18X,3F9.3/1H )                      SEAR 490
      WRITE (NOUT,121)K,ITOM1,IO,ITOM2,IO2,                              SEAR 500
     1ITAR1,ITAR2,(AIN(J),J=5,7)                                         SEAR 510
  124 FORMAT(1H 15X,2I5,I8,I5,2F9.3)                                     SEAR 520
      IF(NCD) 130,130,125                                                SEAR 530
  125 WRITE (NOUT,124) ((KD(J,I),J=1,4),(CD(J,I),J=1,2) ,I=1,            SEAR 540
     1NCD)                                                               SEAR 550
  130 DO 135 J=1,4                                                       SEAR 560
      W(1,J)=99.                                                         SEAR 570
  135 W(2,J)=-99.                                                        SEAR 580
      DO 155 I=ITAR1,ITAR2                                               SEAR 590
      T1=FLOAT(I)*100000.                                                SEAR 600
      CALL ATOM(T1,X)                                                    SEAR 610
      IF(NG) 140,145,140                                                 SEAR 620
  140 CALL ERPNT(T1,KFUN)                                                SEAR 630
      GO TO 600                                                          SEAR 640
  145 X(4)=X(1)-X(2)                                                     SEAR 650
      DO 155 J=1,4                                                       SEAR 660
      TEM=X(J)                                                           SEAR 670
      IF(W(2,J)-TEM) 148,150,150                                         SEAR 680
  148 W(2,J)=TEM                                                         SEAR 690
  150 IF(TEM-W(1,J)) 152,155,155                                         SEAR 700
  152 W(1,J)=TEM                                                         SEAR 710
  155 CONTINUE                                                           SEAR 720
      KFUN2=MOD(KFUN,10)                                                 SEAR 730
      GO TO (165,165,160,156,165,165),KFUN2                              SEAR 740
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES TRICLINIC BOX *****       SEAR 750
  156 DO 158 J=1,3                                                       SEAR 760
  158 DX(J)=AIN(J+4)                                                     SEAR 770
      GO TO 170                                                          SEAR 780
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES RECTANGULAR BOX *****     SEAR 790
  160 DO 162 J=1,3                                                       SEAR 800
      DX(J)=0.                                                           SEAR 810
      DO 162 I=1,3                                                       SEAR 820
  162 DX(J)=DX(J)+ABS(REFV(J,I)*AIN(I+4))                                SEAR 830
      GO TO 170                                                          SEAR 840
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES DMAX SPHERE *****         SEAR 850
  165 T1=1.-A(4)*A(4)-A(5)*A(5)-A(6)*A(6)+2.*A(4)*A(5)*A(6)              SEAR 860
      DO 168 J=1,3                                                       SEAR 870
  168 DX(J)=SQRT((1.-A(J+3)**2)/T1)*DMAX/A(J)                            SEAR 880
C     ***** START SEARCH AROUND REFERENCE ATOMS *****                    SEAR 890
  170 LIST=0                                                             SEAR 900
      LAST=0                                                             SEAR 910
      M1=ITOM1                                                           SEAR 920
      N1=ITOM2                                                           SEAR 930
      IF(KFUN2-5) 186,172,172                                            SEAR 940
C     ***** CONVOLUTE AND REITERATIVE CONVOLUTE INSTRUCTIONS *****       SEAR 950
  172 IF(LATM) 174,174,176                                               SEAR 960
C     ***** FAULT, NO ENTRIES IN ATOMS LIST *****                        SEAR 970
  174 NG=12                                                              SEAR 980
      CALL ERPNT(0.,KFUN)                                                SEAR 990
      GO TO 600                                                          SEAR1000
C     ***** CHECK FOR REFERENCE ATOMS IN ATOMS LIST *****                SEAR1010
  176 IF(LATM-LAST) 600,600,177                                          SEAR1020
  177 LIST=LAST                                                          SEAR1030
      LAST=LATM                                                          SEAR1040
  178 LIST=LIST+1                                                        SEAR1050
      IF(LAST-LIST) 505,180,180                                          SEAR1060
  180 T1=ATOMS(1,LIST)                                                   SEAR1070
      ITOM=T1/100000.                                                    SEAR1080
      IF(ITOM-ITOM1) 178,184,182                                         SEAR1090
  182 IF(ITOM2-ITOM) 178,184,184                                         SEAR1100
  184 SYITOM=AMOD(T1,100000.)                                            SEAR1110
      SYITO2=SYITOM                                                      SEAR1120
      M1=ITOM                                                            SEAR1130
      N1=ITOM                                                            SEAR1140
C     ***** SET INITIAL RUN PARAMETERS *****                             SEAR1150
  186 M2=AMOD(SYITOM,100.)                                               SEAR1160
      M5=AMOD(SYITOM/100.,1000.)                                         SEAR1170
      M3=M5/100                                                          SEAR1180
      M4=MOD(M5/10,10)                                                   SEAR1190
      M5=MOD(M5,10)                                                      SEAR1200
C     ***** SET TERMINAL RUN PARAMETERS *****                            SEAR1210
      N2=AMOD(SYITO2,100.)                                               SEAR1220
      N5=AMOD(SYITO2/100.,1000.)                                         SEAR1230
      N3=N5/100                                                          SEAR1240
      N4=MOD(N5/10,10)                                                   SEAR1250
      N5=MOD(N5,10)                                                      SEAR1260
C     ***** START SEARCH AROUND REFERENCE ATOMS *****                    SEAR1270
      DO 500 L5=M5,N5                                                    SEAR1280
      DO 500 L4=M4,N4                                                    SEAR1290
      DO 500 L3=M3,N3                                                    SEAR1300
      DO 500 L2=M2,N2                                                    SEAR1310
      DO 500 ITOM=M1,N1                                                  SEAR1320
      T1=FLOAT(ITOM)*100000.+FLOAT(L3*10000+L4*1000+L5*100+L2)           SEAR1330
      CALL ATOM(T1,Y)                                                    SEAR1340
      IF(NG) 188,190,188                                                 SEAR1350
  188 CALL ERPNT(T1,KFUN)                                                SEAR1360
      GO TO 500                                                          SEAR1370
C     ***** K=SYMMETRY EQUIVALENT POSITION *****                         SEAR1380
  190 NUM=0                                                              SEAR1390
      DO 400 K=1,NSYM                                                    SEAR1400
C     ***** SUBTRACT SYMMETRY TRANSLATION FROM REFERENCE ATOM *****      SEAR1410
      DO 192 J=1,3                                                       SEAR1420
  192 U(J)=Y(J)-TS(J,K)                                                  SEAR1430
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****                SEAR1440
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****      SEAR1450
      DO 200 J=1,3                                                       SEAR1460
      DO 200 L=1,2                                                       SEAR1470
      WW(L,J)=0.0                                                        SEAR1480
      DO 200 I=1,3                                                       SEAR1490
      TEM=FS(I,J,K)                                                      SEAR1500
      IF(TEM) 194,200,196                                                SEAR1510
  194 N=MOD(L,2)+1                                                       SEAR1520
      GO TO 198                                                          SEAR1530
  196 N=L                                                                SEAR1540
  198 WW(L,J)=WW(L,J)+W(N,I)*TEM                                         SEAR1550
  200 CONTINUE                                                           SEAR1560
C     ***** CHECK FOR MIXED INDEX TRANSFORMATION *****                   SEAR1570
      DO 215 J=1,2                                                       SEAR1580
      TEM=FS(1,J,K)                                                      SEAR1590
      IF(TEM+FS(2,J,K)) 215,201,215                                      SEAR1600
  201 IF(TEM) 203,215,207                                                SEAR1610
  203 WW(1,J)=W(2,4)*TEM                                                 SEAR1620
      WW(2,J)=W(1,4)*TEM                                                 SEAR1630
      GO TO 215                                                          SEAR1640
  207 WW(1,J)=W(1,4)*TEM                                                 SEAR1650
      WW(2,J)=W(2,4)*TEM                                                 SEAR1660
  215 CONTINUE                                                           SEAR1670
C     ***** MOVE 4 CELLS AWAY THEN MOVE BACK UNTIL PARALLELEPIPED AROUNDSEAR1680
C         REF ATOM AND BOX AROUND TRANSFORMED ASYM UNIT INTERSECT ***** SEAR1690
      N=0                                                                SEAR1700
      DO 235 J=1,3                                                       SEAR1710
      DO 225 I=1,2                                                       SEAR1720
      N=N+1                                                              SEAR1730
      TT=(U(J)-WW(I,J))*FLOAT(I*2-3)-DX(J)                               SEAR1740
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      TEM=5.0                                                           SEAR1750
  221 TEM=TEM-1.0                                                       SEAR1760
      IF(TEM+TT) 225,225,221                                            SEAR1770
  225 NW(N)=TEM*FLOAT(I*2-3)+5.                                         SEAR1780
C     ***** IF NO POSSIBILITY OF A HIT, GO TO NEXT SYMMETRY OPER *****  SEAR1790
      IF(NW(N)-NW(N-1))400,235,235                                      SEAR1800
  235 CONTINUE                                                          SEAR1810
      LL=NW(1)                                                          SEAR1820
      LU=NW(2)                                                          SEAR1830
      ML=NW(3)                                                          SEAR1840
      MU=NW(4)                                                          SEAR1850
      NL=NW(5)                                                          SEAR1860
      NU=NW(6)                                                          SEAR1870
C     ***** L CELL TRANSLATIONS IN X *****                              SEAR1880
      DO 395 L=LL,LU                                                    SEAR1890
      V(1)=U(1)+FLOAT(L-5)                                              SEAR1900
C     ***** M CELL TRANSLATIONS IN Y *****                              SEAR1910
      DO 395 M=ML,MU                                                    SEAR1920
      V(2)=U(2)+FLOAT(M-5)                                              SEAR1930
C     ***** N CELL TRANSLATIONS IN Z *****                              SEAR1940
      DO 395 NN=NL,NU                                                   SEAR1950
      V(3)=U(3)+FLOAT(NN-5)                                             SEAR1960
C     ***** I = TARGET ATOM *****                                       SEAR1970
      DO 395 I=ITAR1,ITAR2                                              SEAR1980
      DO 250 J=1,3                                                      SEAR1990
      TEM=0.0                                                           SEAR2000
      DO 245 II=1,3                                                     SEAR2010
  245 TEM=TEM+PS(II,J,K)*P(II,I)                                        SEAR2020
C     ***** SEE IF WITHIN PARALLELEPIPED*****                           SEAR2030
      TEM=TEM-V(J)                                                      SEAR2040
      IF(DX(J)-ABS(TEM))395,250,250                                     SEAR2050
  250 X(J)=TEM                                                          SEAR2060
      GO TO (255,255,252,277,255,255),KFUN2                             SEAR2070
C     ***** SEE IF WITHIN MODEL BOX *****                               SEAR2080
  252 CALL VM(X,AAREV,V1(2))                                            SEAR2090
      DO 253 J=2,4                                                      SEAR2100
      IF(AIN(J+3)-ABS(V1(J)))395,253,253                                SEAR2110
  253 CONTINUE                                                          SEAR2120
      GO TO 277                                                         SEAR2130
C     ***** SEE IF WITHIN SPHERE *****                                  SEAR2140
  255 DSQ=VMV(X,AA,X)                                                   SEAR2150
      IF(DMX-DSQ)395,256,256                                            SEAR2160
  256 IF(DSQ-.0001)258,260,260                                          SEAR2170
  258 IF(KFUN-402)395,260,260                                           SEAR2180
  260 TEM=SQRT(DSQ)                                                     SEAR2190
      IF(AIN(8))265,265,261                                             SEAR2200
C     *****SELECT ONLY FIRST ASYMMETRIC UNIT ENCOUNTERED *****          SEAR2210
  261 IF(LATM)265,265,262                                               SEAR2220
  262 ZMIN=FLOAT(I)*100000.                                             SEAR2230
      ZMAX=ZMIN+100000.                                                 SEAR2240
      DO 264 J=1,LATM                                                   SEAR2250
      ZSTO=ATOMS(1,J)                                                   SEAR2260
      IF(ZSTO-ZMIN)264,263,263                                          SEAR2270
  263 IF(ZMAX-ZSTO)264,264,395                                          SEAR2280
  264 CONTINUE                                                          SEAR2290
C     ***** SELECT VECTORS ACCORDING TO CODES IF ANY *****              SEAR2300
  265 IF(NCD)277,277,268                                                SEAR2310
  268 DO 275 J=1,NCD                                                    SEAR2320
  269 IF(ITOM-KD(1,J))275,270,270                                       SEAR2330
  270 IF(KD(2,J)-ITOM)275,271,271                                       SEAR2340
  271 IF(I-KD(3,J))    275,272,272                                      SEAR2350
  272 IF(KD(4,J)-I)    275,273,273                                      SEAR2360
  273 IF(TEM-CD(1,J))  275,274,274                                      SEAR2370
  274 IF(CD(2,J)-TEM)  275,277,277                                      SEAR2380
  275 CONTINUE                                                          SEAR2390
      GO TO 395                                                         SEAR2400
  277 V1(1) = 100000.*FLOAT(I)+FLOAT((1110-L*100-M*10-NN)*100+K)        SEAR2410
      IF(KFUN-402)278,325,325                                           SEAR2420
C     ***** DETERMINE CORRECT POSITION IN SORTED VECTOR TABLE *****     SEAR2430
  278 IF(NUM)317,317,279                                                SEAR2440
  279 DO 315 II=1,NUM                                                   SEAR2450
      TT=S(2,II)-TEM                                                    SEAR2460
      IF(ABS(TT)-0.0001)297,297,281                                     SEAR2470
  281 IF(TT)315,297,283                                                 SEAR2480
C     ***** MOVE LONGER VECTORS TOWARD END OF TABLE *****               SEAR2490
  283 IF(200-NUM)287,287,289                                            SEAR2500
  287 NUM=199                                                           SEAR2510
  289 IJ=NUM                                                            SEAR2520
      DO 295 J=II,NUM                                                   SEAR2530
      S(1,IJ+1)=S(1,IJ)                                                 SEAR2540
      S(2,IJ+1)=S(2,IJ)                                                 SEAR2550
  295 IJ=IJ-1                                                           SEAR2560
      GO TO 319                                                         SEAR2570
C     ***** CHECK FOR DUPLICATE VECTORS IF DISTANCES ARE EQUAL *****    SEAR2580
  297 CALL ATOM(S(1,II),Z)                                              SEAR2590
      DO 305 J=1,3                                                      SEAR2600
      IF(ABS(X(J)+Y(J)-Z(J))-0.0001)305,305,315                         SEAR2610
  305 CONTINUE                                                          SEAR2620
      GO TO 395                                                         SEAR2630
  315 CONTINUE                                                          SEAR2640
      IF(200-NUM)320,320,317                                            SEAR2650
C     ***** STORE THE RESULT IN VECTOR TABLE *****                      SEAR2660
  317 II=NUM+1                                                          SEAR2670
  319 NUM=NUM+1                                                         SEAR2680
      S(1,II)=V1(1)                                                     SEAR2690
      S(2,II)=TEM                                                       SEAR2700
  320 IF(KFUN-106)395,325,325                                           SEAR2710
C     ***** STORE RESULT IN ATOMS TABLE *****                           SEAR2720
  325 DO 330 J=1,3                                                      SEAR2730
  330 V1(J+1)=X(J)+Y(J)                                                 SEAR2740
      CALL STOR                                                         SEAR2750
  395 CONTINUE                                                          SEAR2760
  400 CONTINUE                                                          SEAR2770
C     ***** PRINT OUT DISTANCES *****                                   SEAR2780
  421 FORMAT(1H010X,20HVECTORS FROM ATOM  (I3,1H,I5,1H)6X,8HTO ATOMSI4, SEAR2790
     18H THROUGHI4)                                                     SEAR2800
      IO = AMOD(T1,100000.)                                             SEAR2810
      WRITE (NOUT,421)ITOM,IO,ITAR1,ITAR2                               SEAR2820
      IF(NUM)500,500,423                                                SEAR2830
  423 DO 435 I=1,NUM                                                    SEAR2840
      T2=S(1,I)                                                         SEAR2850
      I1=T2/100000.                                                     SEAR2860
      I2=T2-FLOAT(I1)*100000.                                           SEAR2870
      CALL ATOM(T2,Z)                                                   SEAR2880
      IF(I-1)432,432,434                                                SEAR2890
  427 FORMAT(1H 13X,2(A6,1X),39X,1H(I3,1H,I5,1H)3F7.4,7X,3HD =F6.3)     SEAR2900
  429 FORMAT(1H 13X,2(A6,1X),2(3H  (I3,1H,I5,1H)3F7.4,3X),4X,3HD =F6.3) SEAR2910
  432 WRITE (NOUT,429)CHEM(ITOM),CHEM(I1),ITOM,IO,(Y(J),J=1,3           SEAR2920
     1),I1,I2,(Z(J),J=1,3),S(2,I)                                       SEAR2930
      GO TO 435                                                         SEAR2940
  434 WRITE (NOUT,427)CHEM(ITOM),CHEM(I1),I1,I2,(Z(J),J=1,3),           SEAR2950
     1S(2,I)                                                            SEAR2960
  435 CONTINUE                                                          SEAR2970
C     ***** CALCULATE ANGLES ABOUT REF ATOM IF CODE IS 102 *****        SEAR2980
  437 IF(KFUN-102)500,451,500                                           SEAR2990
  441 FORMAT(1H010X,18HANGLES ARCUND ATOMI5)                            SEAR3000
  451 WRITE (NOUT,441)ITOM                                              SEAR3010
      L=NUM-1                                                           SEAR3020
      IF(L)500,500,457                                                  SEAR3030
  457 DO 465 I=1,L                                                      SEAR3040
      T2=S(1,I)                                                         SEAR3050
      T3=S(2,I)                                                         SEAR3060
      I1=T2/100000.                                                     SEAR3070
      I2=T2-FLOAT(I1)*100000.                                           SEAR3080
      CALL ATOM(T2,X)                                                   SEAR3090
      CALL DIFV(X,Y,U)                                                  SEAR3100
      CALL MV(AA,U,V2)                                                  SEAR3110
      M=I+1                                                             SEAR3120
      DO 465 J=M,NUM                                                    SEAR3130
      T4=S(1,J)                                                         SEAR3140
      J1=T4/100000.                                                     SEAR3150
      J2=T4-FLOAT(J1)*100000.                                           SEAR3160
      CALL ATOM(T4,Z)                                                   SEAR3170
      CALL DIFV(Z,Y,V)                                                  SEAR3180
      F=ARCCOS(VV(V,V2)/(T3*S(2,J)))                                    SEAR3190
      CALL DIFV(X,Z,V3)                                                 SEAR3200
      F1=SQRT(VMV(V3,AA,V3))                                            SEAR3210
  460 FORMAT(1H 13X,3(A6,1X),7X,3(2H (I3,1H,I5,1H)),12X,3HD =F6.3,7X,3HASEAR3220
     1 =F6.2)                                                           SEAR3230
  465 WRITE (NOUT,460)CHEM(I1),CHEM(ITOM),CHEM(J1),I1,I2,ITOM           SEAR3240
     1,IO,J1,J2,F1,F                                                    SEAR3250
  495 CONTINUE                                                          SEAR3260
  500 CONTINUE                                                          SEAR3270
      IF(LAST-LIST)505,505,178                                          SEAR3280
  505 IF(KFUN2-6)600,176,600                                            SEAR3290
  600 IF(KFUN-106)610,605,610                                           SEAR3300
  605 LATM=LATOM                                                        SEAR3310
  610 RETURN                                                            SEAR3320
      END                                                               SEAR3330


      SUBROUTINE SPARE(INST)                                            SPAR  10
C     ***** INSTRUCTION 1201 PRODUCES PUNCHED CARDS WITH POSIT.+THERMAL SPAR  20
C     ***** PARAMETERS FOR ATOMS PLACED IN THE ATOMS LIST BY THE 400    SPAR  30
C     ***** SERIES INSTRUCTIONS                                         SPAR  40
      REAL*8 CHEM                                                       SPAR  50
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    SPAR  60
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)SPAR  70
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      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) SPAR  80
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) SPAR  90
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   SPAR 100
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   SPAR 110
      DIMENSION XLNG(3),XO(3),XT(3)                                     SPAR 120
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   SPAR 130
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD SPAR 140
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1SPAR 150
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   SPAR 160
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                SPAR 170
      REAL*8 CHM                                                        SPAR 180
C     ***** FIRST FIELD ON INSTRUCTION CARD = NO. OF POSITION PARAMETER SPAR 190
C     ***** CARDS TO BE READ BY THIS SUBROUTINE (STANDARD CRPLS FORMAT) SPAR 200
C     ***** THE SEQUENCE OF THESE CARDS NEED NOT BE IDENTICAL WITH      SPAR 210
C     ***** THE ORIGINAL INPUT ATOM DECK SEQUENCE                       SPAR 220
      IF(INST-1201) 100,105,100                                         SPAR 230
  100 NG = 9                                                            SPAR 240
      RETURN                                                            SPAR 250
  105 IF(AIN(1)) 100,100,115                                            SPAR 260
  115 LAST = AIN(1)                                                     SPAR 270
      DO 150 L=1,LAST                                                   SPAR 280
      READ (IN,116) CHM,V2(1),V2(2),(V1(J),J=1,4)                       SPAR 290
  116 FORMAT(A6,3X,6F9.6)                                               SPAR 300
      WRITE (NOUT,117) CHM,V2(1),V2(2),(V1(J),J=1,4)                    SPAR 310
  117 FORMAT(1H0,24X,25HOLD POSITION PARAMETERS  ,A6,4X,6F10.6)         SPAR 320
C     ***** FIND ATOM NUMBER *****                                      SPAR 330
      DO 125 IA=1,NATOM                                                 SPAR 340
      DO 120 J=1,3                                                      SPAR 350
      IF(ABS(V1(J)-P(J,IA))-0.001) 120,120,125                          SPAR 360
  120 CONTINUE                                                          SPAR 370
      IX = IA                                                           SPAR 380
      GO TO 130                                                         SPAR 390
  125 CONTINUE                                                          SPAR 400
      GO TO 150                                                         SPAR 410
C     ***** SEARCH ATOMS LIST FOR ENTRIES WITH ATOM NUMBER IX *****     SPAR 420
  130 IF(LATM) 150,150,131                                              SPAR 430
  131 DO 145 IB=1,LATM                                                  SPAR 440
      T1 = ATOMS(1,IB)                                                  SPAR.450
      IF(IX-INT(T1/100000.)) 145,135,145                                SPAR 460
  135 CALL ATOM(T1,V1)                                                  SPAR 470
      WRITE (NOUT,136) T1,CHM,V2(1),V2(2),(V1(J),J=1,4)                 SPAR 480
  136 FORMAT(1H0,9X,F10.0,5X,25HNEW POSITION PARAMETERS  ,A6,4X,6F10.6) SPAR 490
      I1 = T1                                                           SPAR 500
      PUNCH 137, CHM,V2(1),V2(2),(V1(J),J=1,4),I1                       SPAR 510
  137 FORMAT(A6,3X,6F9.6,9X,I8)                                         SPAR 520
      CALL PAXES(T1,-1)                                                 SPAR 530
      DO 140 I=1,3                                                      SPAR 540
      DO 140 J=1,3                                                      SPAR 550
  140 Q(J,I) = Q(J,I) /.0506605918                                      SPAR 560
      WRITE (NOUT,141) Q(1,1),Q(2,2),Q(3,3),Q(1,2),Q(1,3),Q(2,3)        SPAR 570
  141 FORMAT(1H ,24X,25HNEW THERMAL PARAMETERS   ,6F10.6)               SPAR 580
      PUNCH 142, Q(1,1),Q(2,2),Q(3,3),Q(1,2),Q(1,3),Q(2,3),I1           SPAR 590
  142 FORMAT(6F9.6,18X,I8)                                              SPAR 600
  145 CONTINUE                                                          SPAR 610
  150 CONTINUE                                                          SPAR 620
  300 RETURN                                                            SPAR 630
      END                                                               SPAR 640


      SUBROUTINE STOR                                                   STOR  10
C     ***** STORE IN OR REMOVE FROM ATOMS ARRAY *****                   STOR  20
      REAL*8 CHM                                                        STOR  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    STOR  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)STOR  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) STOR  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) STOR  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   STOR  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   STOR  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     STOR 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   STOR 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD STOR 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1STOR 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   STOR 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                STOR 150
      IF(LATM) 481,481,450                                              STOR 160
  450 IF(500-LATM) 455,455,460                                          STOR 170
  455 IF(NJ2-10) 490,490,460                                            STOR 180
  460 L=LATM                                                            STOR 190
C     ***** CHECK FOR POSITIONAL DUPLICATION *****                      STOR 200
      DO 480 K=1,L                                                      STOR 210
      DO 465 J=2,4                                                      STOR 220
      IF(ABS(V1(J)-ATOMS(J,K))-0.001) 465,465,480                       STOR 230
  465 CONTINUE                                                          STOR 240
      IF(NJ2-10) 490,490,470                                            STOR 250
C     ***** ATOM REMOVAL BY TABLE PUSHDOWN *****                        STOR 260
  470 LATM=LATM-1                                                       STOR 270
      DO 475 I=K,LATM                                                   STOR 280
      DO 475 J=1,4                                                      STOR 290
  475 ATOMS(J,I)=ATOMS(J,I+1)                                           STOR 300
      GO TO 490                                                         STOR 310
  480 CONTINUE                                                          STOR 320
  481 IF(NJ2-10) 482,490,490                                            STOR 330
C     ***** STORE ATOM *****                                            STOR 340
  482 IF(499-LATM) 490,483,485                                          STOR 350
  483 NG=16                                                             STOR 360
      CALL ERPNT (V1(1),400)                                            STOR 370
  485 LATM=LATM+1                                                       STOR 380
      DO 486 J=1,4                                                      STOR 390
  486 ATOMS(J,LATM)=V1(J)                                               STOR 400
  490 RETURN                                                            STOR 410
      END                                                               STOR 420


      SUBROUTINE TMM(X,Y,Z)                                             TMM   10
C     ***** TRANSPOSE(TRANSPOSE(X)*Y)=Z *****                           TMM   20
C     ***** X,Y,Z ARE 3X3 MATRICES *****                                TMM   30
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                    TMM   40
      DO 115 I=1,3                                                      TMM   50
      DO 115 K=1,3                                                      TMM   60
  115 Z(K,I)=X(1,I)*Y(1,K)+X(2,I)*Y(2,K)+X(3,I)*Y(3,K)                  TMM   70
      RETURN                                                            TMM   80
      END                                                               TMM   90


      SUBROUTINE UNIT(X,Z,ITYPE)                                        UNIT  10
      DIMENSION X(3),Y(3),Z(3)                                          UNIT  20
      REAL*8 CHEM                                                       UNIT  30
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    UNIT  40
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,10),CHEM(166),CONT(5),D(3,130)UNIT  50
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3) UNIT  60
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) UNIT  70
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),TS(3,48)   UNIT  80
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   UNIT  90
      DIMENSION XLNG(3),XO(3),XT(3)                                     UNIT 100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   UNIT 110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNC,NATOM,NCD UNIT 120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1UNIT 130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   UNIT 140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                UNIT 150
      Y(1)=X(1)                                                         UNIT 160
      Y(2)=X(2)                                                         UNIT 170
      Y(3)=X(3)                                                         UNIT 180
      IF(ITYPE) 125,125,105                                             UNIT 190
  105 T1=SQRT(Y(1)*Y(1)+Y(2)*Y(2)+Y(3)*Y(3))                            UNIT 200
      GO TO 145                                                         UNIT 210
  125 T1=SQRT(Y(1)*(Y(1)*AA(1,1)+Y(2)*(AA(1,2)+AA(2,1))+Y(3)*(AA(1,3)+A UNIT 220
     1A(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2)))+Y(3)*Y(3)*AA(3UNIT 230
     2,3))                                                              UNIT 240
  145 IF(T1) 155,155,175                                                UNIT 250
  155 NG=5                                                              UNIT 260
      GO TO 300                                                         UNIT 270
  175 Z(1)=Y(1)/T1                                                      UNIT 280
      Z(2)=Y(2)/T1                                                      UNIT 290
      Z(3)=Y(3)/T1                                                      UNIT 300
  300 RETURN                                                            UNIT 310
      END                                                               UNIT 320


      SUBROUTINE VM(X,Y,Z)                                              VM    10
C     TRANSPOSED VECTOR TIMES MATRIX                                    VM    20
C     Z(3)=X(3)*Y(3,3)                                                  VM    30
      DIMENSION X(3),Y(3,3),Z(3)                                        VM    40
      DO 115 J=1,3                                                      VM    50
      Z(J)=0.0                                                          VM    60
      DO 115 I=1,3                                                      VM    70
  115 Z(J)=Z(J)+X(I)*Y(I,J)                                             VM    80
      RETURN                                                            VM    90
      END                                                               VM   100


      FUNCTION VMV(X1,Q,X2)                                             VMV   10
C     TRANSPOSED VECTOR * MATRIX * VECTOR                               VMV   20
C     VMV=X1(3)*Q(3,3)*X2(3)     TO  EVALUATE QUADRATIC OR BILINEAR FORM VMV  30
      DIMENSION X1(3),Q(3,3),X2(3)                                      VMV   40
      T1=0.                                                             VMV   50
      DO 10 J=1,3                                                       VMV   60
   10 T1=T1+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))              VMV   70
      VMV=T1                                                            VMV   80
```

```
      RETURN
      END


      FUNCTION VV(X,Y)
C     TRANSPOSED VECTOR * VECTOR
C     VV=X(3)*Y(3)
      DIMENSION X(3),Y(3)
      VV=X(1)*Y(1)+X(2)*Y(2)+X(3)*Y(3)
      RETURN
      END


      SUBROUTINE XYZ(QA,X,ITYPE)
C     ***** ITYPE .GT.0 CART. COORD. FROM ATOM CODE WORD *****
C     ***** XABSF(ITYPE) .LE.2 FOR WORKING SYSTEM *****
C     ***** XABSF(ITYPE) .GT.2 FOR REFERENCE SYSTEM *****
C     ***** ITYPE .LE.0 USES TRICLINIC COORD. XT *****
      DIMENSION X(3)
      REAL*8 CHEM
      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(8,10),CHEM(166),CONT(5),D(3,130)
      DIMENSION DA(3,3),DP(2,130),EV(3,166),FS(3,3,48),KD(5,10),ORGN(3)
      DIMENSION P(3,166),PA(3,3,166),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(18),TITLE2(18),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,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT
      IT=IABS(ITYPE)-2
      NG1=NG
      NG=0
      IF(ITYPE) 10,10,5
    5 CALL ATOM(QA,XT)
      IF(NG) 30,10,30
   10 T1=0.
      DO 15 J=1,3
      T2=XT(J)-ORGN(J)
      V1(J)=T2
   15 T1=T1+ABS(T2)
      IF(T1-.0001)20,20,40
   20 NG=NG1
   30 DO 35 J=1,3
   35 X(J)=0.
      GO TO 300
   40 IF(IT) 45,45,60
C     ***** RELATIVE TO WORKING SYSTEM *****
   45 DO 55 I=1,3
      T1=0.
      DO 50 J=1,3
   50 T1=T1+V1(J)*AAWRK(J,I)
   55 X(I)=T1*SCAL1
      GO TO 300
C     ***** RELATIVE TO REFERENCE SYSTEM *****
   60 DO 70 I=1,3
      T1=0.
      DO 65 J=1,3
   65 T1=T1+V1(J)*AAREV(J,I)
   70 X(I)=T1*SCAL1
  300 RETURN
      END


      SUBROUTINE CRT(X1,Y1,I1,I2)
C     ***** DUMMY SUBROUTINE TO REPLACE THE CATHODE-RAY-TUBE PACKAGE ***
C     ***** SUBROUTINE CRT IS CALLED BY SUBROUTINES F200 AND DRAW *****
      RETURN
      END


      SUBROUTINE IDAY(H2)
C     ***** DUMMY FOR ORNL LOCAL SUBROUTINE CALLED BY F200 FOR CRT IDENT
C     ***** IDAY OBTAINS DATE (8 BCD CHARACTERS) FROM OPERATING SYSTEM
      RETURN
      END
```

```
      SUBROUTINE JOBNUM(H1)
C     ***** DUMMY FOR ORNL LOCAL SUBROUTINE CALLED BY F200 FCR CRT IDENT
C     ***** JOBNUM OBTAINS USERS JOB NUMBER (4 BCD CHARACTERS) *****
      RETURN
      END
```

```
 CUBANE  E.B.FLEISCHER   1964  J.A.C.S.  86,3889
    5.34      5.34      5.34     72.26     72.26     72.26
          0  1  0  0                 0  0  1  0                 0  0  0  1
          0  0  0  1                 0  1  0  0                 0  0  1  0
          0  0  1  0                 0  0  0  1                 0  1  0  0
          0 -1  0  0                 0  0 -1  0                 0  0  0 -1
          0  0  0 -1                 0 -1  0  0                 0  0 -1  0
1         0  0 -1  0                 0  0  0 -1                 0 -1  0  0
  C1                           -.18711   .19519   .10706        0
  .04100    .04250    .04500  -.00420  -.01420  -.00510         0
  C2                            .11546   .11546   .11546        0
  .04680    .04680    .04680  -.01430  -.01430  -.01430         0
  H1                           -.32460   .34680   .18480        0
     .10                                                        7
  H2                            .21000   .21000   .21000        0
     .10                                                        7
 ORGN                                0        0        0        0
1                                                               0
  3   101  155501        2         1         4       3.61
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****
  3   102  155501        2         1         4       1.8
***** FIND COVALENT BONDS ANC BOND ANGLES AROUND CARBONS *****
  3   201
***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****
  3   301      11.       11.       30.       1.5
***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****
  3   303
***** ELIMINATE ALL RETRACING *****
  3   402  555501        5         1         4       3.2
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****
  3   501  555501  255501  155501  255501  155502                   0
***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****
  3   502        2       25.         1       28.
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****
  3   604        0         0         0      1.54
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **
  3   503        2       2.7
***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****
  3  1101
***** START SAVE SEQUENCE *****
  2   511        0
  3        1  4  1  4  4   0.9   1.6   .04
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT
  1   715        4         0         1         0       .20       .60      .70
  3                                  1         2
***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
  1   712                                              .20       .35      .40
  3                                  3         4
***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****
  2   812
  3        1  4  1  4  4   0.9   1.6   .04
***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A
  3   906  155504  155503        0         0       .15         0      -.4
***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****
  3   916  255504  155505        0         0       .15         0      -.4
***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ***4
  3   902  555501        0         0       1.0       .25         0       0
                                 CUBANE
  3  1102
***** END OF SAVE SEQUENCE *****
  3   202       9.
***** ADVANCE PLOTTER 9 INCHES ALONG X *****
  3   503        2      -2.7
***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****
  3  1103
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****
  3   202      20.
***** ADVANCE PLOTTER 20 INCHES *****
  3   202
***** ADD DUMMY PLOT TO MAGNETIC TAPE *****
    -1
```

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