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OR TEP:

A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Carroll K. Johnson

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CHEMISTRY DIVISION

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Carroll K. Johnson

JUNE 1965

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CONTENTS

ABSTRACT 1

1. INTRODUCTION 1

2. GENERAL PRINCIPLES AND PROCEDURES 2

2.1 Summary Table of Instructions 2

2.2 Programming a Nonstereoscopic Illustration for OR TEP 6
2.2.1 General Comments on Automated Graphics 6
2.2.2 Preliminary Graphical Details 6
2.2.3 Composing the Illustration 7
2.2.4 Drawing the Illustration 7
2.2.5 Terminating the Drawing of the Illustration 7

2.3 Programming a Stereoscopic Illustration for OR TEP 8
2.3.1 Stereoscopic Rotations 8
2.3.2 Repeating a Sequence of Operations 8

2.4 Drawing the Cubane Structure: An Example 9
2.4.1 Data Input for Cubane 9
2.4.2 Analysis of Structure 11
2.4.3 Programming the Cubane Illustration 11
2.4.4 Stereoscopic Illustration of Cubane 15
2.4.5 Listing of Sample Input and Output 17

3. DETAILED OPERATING INSTRUCTIONS 28

3.1 Definitions 28
3.1.1 Atom Designator Code (ADC) and Addressable Point 28
3.1.2 Vector Designator Code (VDC) 28
3.1.3 Atom Designator Run (ADR) 28
3.1.4 Atom Number Run (ANR) 28
3.1.5 Vector Search Code (VSC) 29
3.1.6 Sphere of Enclosure 29
3.1.7 Box of Enclosure 29
3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems 29
3.1.9 Prime Parameters and Primer Constants 30

3.2 Crystal Structure Data Input 30
3.2.1 Title Card 30
3.2.2 Cell Parameter Card 30
3.2.3 Symmetry Cards ($1 \leqq NSYM \leqq 48$) 30
3.2.4 Atom Parameter Cards ($1 \leqq NATOM \leqq 200$) 31

3.3 Instruction Input 33
3.3.1 Instruction Cards 34
3.3.2 Structure Analysis Instructions (100 Series) 35
3.3.3 Plotter Control Instructions (200 Series) 37
3.3.4 Plot Boundary Instructions (300 Series) 37
3.3.5 Atom List Instructions (400 Series) 39
3.3.6 Orienting Instructions (500 Series) 40
3.3.7 Positioning and Scaling Instructions (600 Series) 42
3.3.8 Atom Plotting Instructions (700 Series) 44
3.3.9 Bond Plotting Instructions (800 Series) 47
3.3.10 Label Plotting Instructions (900 Series) 49

3.3.11 Saved Sequence Instructions (1100 Series) 51
3.3.12 Job Termination Instructions (Negative Series) 51

3.4 List of Fault Indicators 52

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS) 53

4.1 Graphic-Computational Methods 53
4.1.1 Drawing Ellipsoids 53
4.1.2 Drawing Bonds 55

4.2 OR TEP Subprograms 57
4.2.1 Mainstream Subprograms 57
4.2.2 Subsidiary Subprograms 58
4.2.3 Arithmetic Subprograms 59
4.2.4 Plotting Subprograms for the CalComp Plotter 60

4.3 Adapting OR TEP to Other Equipment Configurations 63
4.3.1 OR TEP Source Deck Differences for the IBM 7090 and the CDC 1604A 63
4.3.2 Magnetic Tape Logical Number Assignments 64
4.3.3 Plotter Systems Other than the CalComp 580 64
4.3.4 Computing Systems Other than the CDC 1604A and IBM 7090 64

4.4 Addition of New OR TEP Instructions 64

4.5 Glossary of Symbols in OR TEP Common, with Array Dimensions 65

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS 68

5.1 Probability Density Function (pdf) of a Trivariate Normal Distribution 68

5.2 Equiprobability Ellipsoids 69

5.3 Characteristic Function (c.f.) of a Trivariate Normal Distribution 69

5.4 Principal Axis Transformation 71

6. EXAMPLES OF ILLUSTRATIONS THAT HAVE BEEN PRODUCED WITH OR TEP 73

6.1 Nonstereoscopic Drawings Showing Thermal Motion 73
6.1.1 Comparison of Graphical Representations of Thermal Motion 73
6.1.2 Thermal Ellipsoids Derived from Independent Sets of Diffraction Data 73
6.1.3 Thermal Motion in Molecules Not Related by Crystallographic Symmetry 73

6.2 Stereoscopic Drawings of Crystal Structure 74
6.2.1 Thermal Ellipsoids Derived from Neutron Studies 74
6.2.2 Thermal Ellipsoids Derived from X-Ray Studies 74
6.2.3 Crystal Structure Packing Diagrams 75

6.3 Helical Structures 76

7. FORTRAN LISTING OF OR TEP 88

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

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

1. INTRODUCTION

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

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

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

Stereoscopic crystal structure illustrations were used quite extensively in the 1920's and 1930's, particularly by M. von Laue and R. von Mises in their beautifully done two-volume series of stereoscopic drawings.[1] More recently, computer techniques were applied in making crystal structure stereoscopic pictures by W. R. 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 FORTRAN listing.

2. GENERAL PRINCIPLES AND PROCEDURES

2.1 Summary Table of Instructions

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

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

---

[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	DMAX (A)	–	–
Dist. + ang.	0 or 2	102	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Princ. axes	–	103	–	–	–	–	–	–	–
Plotter control									
Initialize	–	201	–	–	–	–	–	–	–
Advance and term.	–	202	X(IN)	Y(IN)	–	–	–	–	–
Plot boundary									
Dimensions	–	301	X(IN)	Y(IN)	VIEW(IN)	BRDR(IN)	–	–	–
Title rotation	–	302	THETA (°)	–	–	–	–	–	–
Retrace displace	–	303	X(IN)	–	–	–	–	–	–
Atoms list									
Run add	–	401	From	(–) to	From	(–) to	....	....	....
Run subtract	–	411	From	(–) to	From	(–) to	....	....	....
Sphere add	0 or 2	402	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Sphere subtract	0 or 2	412	ORG 1	ORG 2	TAR 1	TAR 2	DMAX (A)	–	–
Box add	–	403	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Box subtract	–	413	ORG 1	ORG 2	TAR 1	TAR 2	A/2 (A)	B/2 (A)	C/2 (A)
Zero atoms list	–	410	–	–	–	–	–	–	–
Cartesian system									
Definition	–	501	ORGN	V1A	V1B	V2A	V2B	–	–
Rotate reference	–	502	Axes No.	Rotate (°)	Axes No.	Rotate (°)	....	....	....
Rotate working	–	503	Axes No.	Rotate (°)	–	–	–	–	–

Table 2.1 (continued)

Function	1–3	4–9	10–18	19–27	28–36	37–45	46–54	55–63	64–72
Center and scale									
Explicit	–	601	XO (IN)	YO (IN)	SCAL1	SCAL2	–	–	–
Scale only	–	602	XO (IN)	YO (IN)	–	SCAL2	–	–	–
Center only	–	603	–	–	SCAL1	SCAL2	–	–	–
Center and scale	–	604	–	–	–	SCAL2	–	–	–
I. P. and I. S.[a]	–	611	ΔXO (IN)	ΔYO (IN)	ΔSCAL1	SCAL2	–	–	–
I. P. and scale	–	612	ΔXO (IN)	ΔYO (IN)	–	SCAL2	–	–	–
I. S. and center	–	613	–	–	ΔSCAL1	SCAL2	–	–	–
Ellipsoids									
Shaded football	0 or 1	701	–	–	–	–	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)	–	–	A0 (IN)	A1 (IN)	–	–	–	–	–
Football	0 or 1	702	(same as 701)						
Open model	0 or 1	703	(same as 701)						
Boundary only	0 or 1	704	(same as 701)						
Other types	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	SYM HGT	PAR-OFF[b]	PER-OFF[c]
(Format No. 1 trailer card)	–		A0 (IN)	A1 (IN)					
As above except no	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.)	0 or 1	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	–	–	–	–	–	–	–

[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.).

Table 2.1 (continued)

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

2.2 Programming a Nonstereoscopic Illustration for OR TEP

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

2.3 Programming a Stereoscopic Illustration for OR TEP

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

2.3.1 Stereoscopic Rotations. – In general, one member of a detailed stereoscopic illustration cannot be drawn completely independent of the other member of the pair because certain features (e.g., which octant of an ellipsoid is shaded) must be done identically in the two drawings. In OR TEP the "stereoscopically sensitive decisions" are handled by using two Cartesian coordinate systems: the reference Cartesian system and the working Cartesian system (see 3.1.8). The steps involved in picture composition (see 2.2.3) and the stereoscopically sensitive decisions are always based on the reference system, but the drawing of the illustration (see 2.2.4) is always based on the working system. A stereoscopic rotation is simply a rotation of the working system *from the reference system* about the axis which is vertical while viewing the final result. For example, a nominal rotation of +3° 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 3.3.3)

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

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

---

[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 3.3.4.1): FORMAT (A6, 3X,5F9.6,F9.0)

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

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

Card No.									
(9)		C1				−.18711	.19519	.10706	0
(10)	0		.04100	.04250	.04500	−.00420	−.01420	−.00510	0
(11)		C2				.11546	.11546	.11546	0
(12)	0		.04680	.04680	.04680	−.01430	−.01430	−.01430	0

Atoms 3 and 4 are entered with positional parameters type 0 and with dummy sphere temperature factors (type 7) 0.1 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 last paragraph of 3.2.4.2). This could also be entered with type 7 as were atoms 3 and 4.

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

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

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

Card No.

(19) 101 155501 2 1 4 3.61

Atoms 1 through 2 of 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-in. margin to give a total working area of 9 by 9 in. A 24-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 24 1

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

(23) 303 0

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

Card No.

(24) 402 555501 5 1 4 3.2

(a) (b) (c)

where the several parts designate:

(a) a run of origin atom (center of sphere) from atom 5 to atom 5 in symmetry position 55501 (that is, in this example, a single sphere),

(b) a run of target atom from atom 1 to atom 4, and

(c) a sphere radius of 3.2 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

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

(27) 503 2 3.0

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

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

(28) 604 0 0 0 1.54

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

Card No.

(29) 611 0 0 .9 0

This completes the composition of the illustration.

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

The 1101 instruction starts the saved sequence.

(30) 1101

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

(31) 412 555501 5 3 4 3.2

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

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

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

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

(33) 410

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

Card No.

(34) 401 355501 – 455506

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

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

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

(36) 402 555501 5 1 4 3.2

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

(37) 2 812

(38) 0 $\underbrace{1 \quad 4}_{(a)}$ $\underbrace{1 \quad 4}_{(b)}$ $\underbrace{4}_{(c)}$ $\underbrace{.9 \quad 1.6}_{(d)}$ $\underbrace{.04}_{(e)}$

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.

(39) 906 155504 155503 0 0 .15 0 –.4

(40) 916 255504 155505 0 0 .15 0 –.4

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

Card No.									
(41)	3	902	555501	0	0	1.	.25	0	0
(42)				CUBANE					

The saved sequence can now be terminated.

(43) 1102

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

(44) 202 9

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

(45) 503 2 −3.0

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

(46) 1103

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

(47) 202 20

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

(48) 202 0

Finally we terminate the job and exit from the program.

(49) −1

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

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

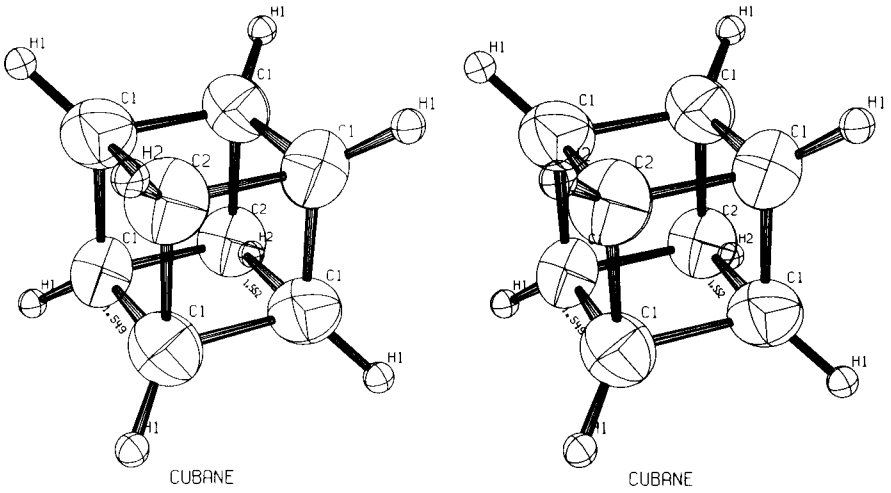

Fig. 2.1. The Sample Figure Cubane Before Retouching.

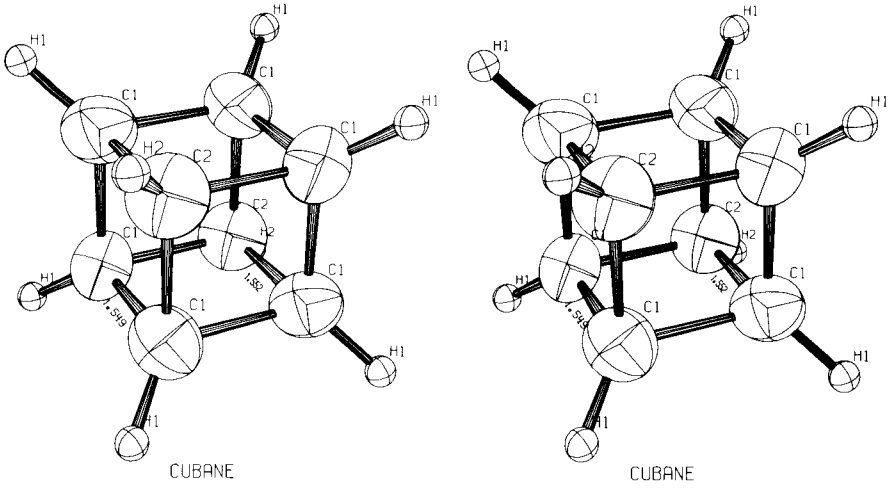

Fig. 2.2. The Sample Figure Cubane After Retouching.

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

```
  CUBANE (E.B.FLEISCHER  (1964) J.A.C.S  86,3889)                          EXAM0010
     5.34      5.34      5.34     72.26     72.26     72.26                 EXAM0020
               0  1  0  0                0  0  1  0                0  0  0  1EXAM0030
               0  0  0  1                0  1  0  0                0  0  1  0EXAM0040
               0  0  1  0                0  0  0  1                0  1  0  0EXAM0050
               0 -1  0  0                0  0 -1  0                0  0  0 -1EXAM0060
               0  0  0 -1                0 -1  0  0                0  0 -1  0EXAM0070
1              0  0 -1  0                0  0  0 -1                0 -1  0  0EXAM0080
  C1                            -.18711   .19519   .10706         0         EXAM0090
   .04100    .04250    .04500  -.00420  -.01420  -.00510         0         EXAM0100
  C2                             .11546   .11546   .11546         0         EXAM0110
   .04680    .04680    .04680  -.01430  -.01430  -.01430         0         EXAM0120
  H1                            -.32460   .34680   .18480         0         EXAM0130
      .10                                                          7         EXAM0140
  H2                             .21000   .21000   .21000         0         EXAM0150
      .10                                                          7         EXAM0160
 ORGN                                 0        0        0         0         EXAM0170
1                                                                 0         EXAM0180
  3   101   155501        2        1        4      3.61                    EXAM0190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****         EXAM0200
  3   102   155501        2        1        4      1.8                     EXAM0210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****             EXAM0220
  3   201                                                                 EXAM0230
***** INITIALIZE CALCOMP PLOT PACKAGE *****                                EXAM0240
  3   301      11.      11.      24.       1.                             EXAM0250
***** 11X11 BOUNDARY, 9X9 INSIDE 1 INCH MARGIN, VIEW FROM 24 INCHES ****EXAM0260
  3   303        0                                                        EXAM0270
***** ELIMINATE ALL RETRACING *****                                        EXAM0280
  3   402   555501        5        1        4      3.2                     EXAM0290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5 *****             EXAM0300
  3   501   555501   255501   155501   255501   155502                   0EXAM0310
***** ORGN AT DUMMY ATOM 5, VECTORS ALONG 2 EDGES OF CUBANE *****          EXAM0320
  3   502        2      25.        1      28.                             EXAM0330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT X *****             EXAM0340
  3   503        2      3.0                                               EXAM0350
***** STEREO ROTATION OF 3.0 DEGREES ABOUT Y FOR LEFT EYE *****            EXAM0360
  3   604        0        0        0     1.54                             EXAM0370
***** AUTO SCALE AND POSITION TO 9X9. 50 PERCENT PROBABILITY ELLIPSOIDS EXAM0380
  3   611        0        0       .9        0                             EXAM0390
***** SHRINK SCALE BY 10 PERCENT FOR SAFETY *****                          EXAM0400
  3  1101                                                                 EXAM0410
***** START SAVE SEQUENCE *****                                            EXAM0420
  3   412   555501        5        3        4      3.2                     EXAM0430
***** ELIMINATE HYDROGENS WITH ENCLOSER SPHERE ELIMINATION *****           EXAM0440
  3   715        4        0        1        0      .20      .60      .70EXAM0450
***** SPECIAL MODEL WITH .2 IN. CHEM SYMBOLS OFFSET .60 ,.70 IN. *****    EXAM0460
  3   410                                                                 EXAM0470
***** ZERO ATOMS ARRAY, THIS STRUCTURE IS TO BE DRAWN PIECEMEAL *****     EXAM0480
  3   401   355501  -455506                                               EXAM0490
***** REPLACE HYDROGENS ONLY WITH AN ATOM DESIGNATOR RUN *****             EXAM0500
  3   712                                                 .2      .35      .40EXAM0510
***** SOLID MODEL WITH .2 INCH CHEM SYMBOLS OFFSET .35,.40 INCH *****     EXAM0520
  3   402   555501        5        1        4      3.2                     EXAM0530
***** ENCLOSER SPHERE WITH COMPLETE MODEL *****                            EXAM0540
  2   812                                                                 EXAM0550
  3        1  4  1  4  4     .9   1.6   .04                               EXAM0560
***** TYPE 4 BONDS,.04 A MAX RADIUS, ALL VECTORS .9 TO 1.6 A LONG ***** EXAM0570
  3   906   155504   155503        0        0      .15        0      -.4EXAM0580
***** LABEL UNIQUE C-C BONDS .   CAPTION # CUBANE *****                    EXAM0590
      916   255504   155505        0        0      .15        0      -.4EXAM0600
  3   902   555501        0        0      1.0      .25        0        0EXAM0610
                                CUBANE                                    EXAM0620
  3  1102                                                                 EXAM0630
***** END OF SAVE SEQUENCE *****                                          EXAM0640
  3   202       9.                                                        EXAM0650
```

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

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

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

DIRECT CELL PARAMETERS
     A            B            C            ALPHA        BETA         GAMMA
 5.340000     5.340000     5.340000        72.260       72.260       72.260
                                     COSINE 0.30469811   0.30469811   0.30469811

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

SYMMETRY TRANSFORMATIONS
    NO.          TRANSFORMED X                    TRANSFORMED Y                    TRANSFORMED Z
     1     0.     1. X  0. Y  0. Z     0.          0. X  1. Y  0. Z     0.          0. X  0. Y  1. Z
     2     0.     0. X  0. Y  1. Z     0.          1. X  0. Y  0. Z     0.          0. X  1. Y  0. Z
     3     0.     0. X  1. Y  0. Z     0.          0. X  0. Y  1. Z     0.          1. X  0. Y  0. Z
     4     0.    -1. X  0. Y  0. Z     0.          0. X -1. Y  0. Z     0.          0. X  0. Y -1. Z
     5     0.     0. X  0. Y -1. Z     0.         -1. X  0. Y  0. Z     0.          0. X -1. Y  0. Z
     6     0.     0. X -1. Y  0. Z     0.          0. X  0. Y -1. Z     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.         7.
 4   H2     0.210000  0.210000  0.210000       0.100000  -0.        -0.        -0.        -0.        -0.         7.
 5  ORGN    0.        0.        0.            -0.        -0.        -0.        -0.        -0.        -0.         0.

NO. ATOM        X          Y          Z            RMSD 1     RMSD 2     RMSD 3
 1   C1    -0.187110  0.195190  0.107060       0.204899   0.239856   0.255794
 2   C2     0.115460  0.115460  0.115460       0.205704   0.247733   0.247733
 3   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.             0.100000   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  -0.5990827E-01  -0.4722319E-01          0.5340000E 01   0.4470348E-07   0.2980232E-07
  0.              0.1966152E-00  -0.4722319E-01          0.1627088E 01   0.5086078E 01   0.2980232E-07
  0.              0.              0.2022067E-00          0.1627088E 01   0.1187798E 01   0.4945434E 01

(((((  INSTRUCTION  101  )))))
 0.1555010E 06  0.2000000E 01  0.1000000E 01  0.4000000E 01  0.3610000E 01 -0.          -0.

***** FIND ALL NEIGHBOR ATOMS AROUND 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    2      1    4                        3.610   -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                                          (  2,56504)-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                                          (  2,55504)-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                                          (  3,55506)-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                                          (  1,56504) 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  0.1800000E 01 -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    2      1    4                          1.800   -0.      -0.

VECTORS FROM ATOM  (  1,55501)       TO ATOMS    1 THROUGH   4
     C1      H1    (  1,55501)-0.1871 0.1952 0.1071      (  3,55501)-0.3246 0.3468 0.1848        D # 1.012
     C1      C1                                          (  1,55505)-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)                                124.69
     H1      C1      C1            (  3,55501) (  1,55501) (  1,55506)                                127.16
     H1      C1      C2            (  3,55501) (  1,55501) (  2,55501)                                123.52
     C1      C1      C1            (  1,55505) (  1,55501) (  1,55506)                                 89.60
     C1      C1      C2            (  1,55505) (  1,55501) (  2,55501)                                 90.48
     C1      C1      C2            (  1,55506) (  1,55501) (  2,55501)                                 90.48

VECTORS FROM ATOM  (  2,55501)       TO ATOMS    1 THROUGH   4
     C2      H2    (  2,55501) 0.1155 0.1155 0.1155      (  4,55501) 0.2100 0.2100 0.2100        D # 1.109
     C2      C1                                          (  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)                                125.66
     H2      C2      C1            (  4,55501) (  2,55501) (  1,55502)                                125.66
     H2      C2      C1            (  4,55501) (  2,55501) (  1,55503)                                125.66
     C1      C2      C1            (  1,55501) (  2,55501) (  1,55502)                                 89.44
     C1      C2      C1            (  1,55501) (  2,55501) (  1,55503)                                 89.44
     C1      C2      C1            (  1,55502) (  2,55501) (  1,55503)                                 89.44

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

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

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

***** 11X11 BOUNDARY, 9X9 INSIDE 1 INCH MARGIN, VIEW FROM 24 INCHES ****

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

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

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

RETRACE DISPLACEMENT # 0.     INCH
```

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

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

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

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


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

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

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

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

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR         Y VECTOR         Z VECTOR
  -0.1950172E-00  -0.5332417E-01   0.3517815E-02          -0.5161574E 01   0.2128974E-00   0.1352193E 01
   0.5138884E-01   0.4031208E-02   0.1955262E-00          -0.2760937E-00   0.1350080E 01   0.5159133E 01
  -0.5414101E-02   0.1954783E-00  -0.5144393E-01          -0.1402323E 01   0.5145891E 01   0.2624691E-00

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

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

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES                POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR         Y VECTOR         Z VECTOR
  -0.1752589E-00  -0.8727205E-01   0.5055148E-01          -0.4106513E 01  -0.1411455E 01   0.3108044E 01
   0.1292070E-00  -0.6943834E-01   0.1391812E-00           0.1930118E 01  -0.1057867E 01   0.4865301E 01
  -0.2664798E-01   0.1934115E-00   0.5262520E-01          -0.1160012E 01   0.4153645E 01   0.3149160E 01

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

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

ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES                  POST-FACTOR TRANSFORMATION MATRIX
     X VECTOR         Y VECTOR         Z VECTOR
  -0.1723731E-00  -0.8727205E-01   0.5965454E-01          -0.3938223E 01  -0.1411455E 01   0.3318703E 01
   0.1363141E-00  -0.6943834E-01   0.1322283E-00           0.2182103E 01  -0.1057867E 01   0.4757619E 01
  -0.2385727E-01   0.1934115E-00   0.5394772E-01          -0.9936078E 00   0.4153645E 01   0.3205554E 01

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

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

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

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

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

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

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

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

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

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

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

412  555501    5      3    4                       3.200   -0.      -0.


VECTORS FROM ATOM  (  5,55501)      TO ATOMS   3 THROUGH   4

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

((((( INSTRUCTION  812 )))))
      -0.          -0.          -0.          -0.          -0.          -0.          -0.
         1  4  1  4  4    0.90000    1.60000    0.04000   -0.        -0.        -0.        -0.        -0.

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

      BOND SELECTION CODES

      (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
      (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
          1    4       1    4       4  0.90  1.60   0.040  -0.     -0.     -0.     -0.       -0.
      FAULT NG # 14   455504.   800


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

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

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

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

                                     CUBANE

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

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

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

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

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

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

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

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

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

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

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

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

412  555500    4      3    4                        3.200    -0.       -0.


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

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

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

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

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

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

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

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

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

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

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

(((((  INSTRUCTION  402 )))))
       0.5555010E 06  0.5000000E 01  0.9999999E 00  0.4000000E 01  0.3200000E 01 -0.            -0.

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

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

      402  555500    4      1    4                          3.200   -0.       -0.


      VECTORS FROM ATOM  (  5,55500)      TO ATOMS   1 THROUGH   4

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

(((((  INSTRUCTION  812 )))))
      -0.            -0.            -0.            -0.            -0.            -0.            -0.
         1  4  1  4  4    0.90000    1.60000    0.04000   -0.         -0.         -0.         -0.         -0.

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

      BOND SELECTION CODES

      (SEQUENCE(A))(SEQUENCE(B)) (BOND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(DIGITS)
      (  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIUS)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER)
          1    4       1    4       4  0.90  1.60   0.040  -0.     -0.     -0.     -0.       -0.
      FAULT NG # 14   455504.   800


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

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

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

(((((  INSTRUCTION  902 )))))
       0.5555010E 06  0.             0.             0.9999999E 00  0.2500000E-00  0.             0.

                                        CUBANE
```

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

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

(((((  INSTRUCTION   202  )))))
       0.20000000E 02 -0.            -0.            -0.            -0.            -0.            -0.

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

(((((  INSTRUCTION   202  )))))
       0.             -0.            -0.            -0.            -0.            -0.            -0.

      *****  ADDS DUMMY PLOT TO MAGNETIC TAPE  *****

(((((  INSTRUCTION    -1  )))))
```

3. DETAILED OPERATING INSTRUCTIONS

3.1 Definitions

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

3.1.1 Atom Designator Code (ADC) and Addressable Point. – In order to specify a particular atom in the crystal within a reasonable distance from the crystallographically defined origin, the following five-component *a*tom *d*esignator 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* ($0 \leqq AN \leqq NATOM \leqq 200$) = the sequential number of the atom in the input list of atoms in the asymmetric unit, which contains NATOM atoms. Atom zero is not in the input atom list but refers to the crystal origin point (0., 0., 0.).

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. In certain cases 0,0,0 is permitted in place of 5,5,5; however, a mixed translation designation such as 0,5,5 is not permitted.

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.

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 $9 \times 9 \times 9$ block of unit cells.

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

Example: 253704 263704 is a vector along the positive **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 rectangular parallelepiped which can be centered about any addressable point and assigned arbitrary orientation and dimensions. This "box of enclosure" can have a *complete population* or a *partial population* as described for the sphere of enclosure (3.1.6). However, vector screening is not allowed with the box of enclosure.

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

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

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 30.0 in. for x maximum and 11.0 in. for y maximum, and the overall scale for plotting (instruction 600 series) is set at 1.0 in./A. If the value assigned to a particular constant by the primer routine is satisfactory, the user does not have to reset this constant with OR TEP instructions.

3.2 Crystal Structure Data Input

3.2.1 Title Card. – FORMAT (12A6)

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

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

Columns	Type A	Type B	Type C	Type D
1–9	**a** (A)	**a** (A)	**a*** (A^{-1})	**a*** (A^{-1})
10–18	**b** (A)	**b** (A)	**b*** (A^{-1})	**b*** (A^{-1})
19–27	**c** (A)	**c** (A)	**c*** (A^{-1})	**c*** (A^{-1})
28–36	α (deg)	cos 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[3]

[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.

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

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

$$X_1 = T_1 + S_{11} X + S_{12} Y + S_{13} Z ,$$
$$Y_1 = T_2 + S_{21} X + S_{22} Y + S_{23} Z ,$$
$$Z_1 = T_3 + S_{31} X + S_{32} Y + S_{33} Z ,$$

or in matrix notation

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

where

$\mathbf{T} = (T_1, T_2, T_3)$ 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 $\leqq$ NATOM $\leqq$ 200). – Two cards are required for each input atom. The first contains the chemical symbol and positional parameters, and the second contains temperature factor

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

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

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

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

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

Columns						
1	A sentinel $\neq 0$ for last atom only					
	Type 0,1,2,3	Type 4,5	Type 6		Type 7	
2–9	b_{11}	U_{11}	B	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	4,5	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 0–3, are defined as follows: The complete temperature factor is

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

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

type 1: Base = e, C = 1;

type 2: Base = 2, C = 2;

type 3: Base = 2, C = 1.

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

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

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

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

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, $(\text{VDC}_1 \times \text{VDC}_2)$, and $\text{VDC}_1 \times (\text{VDC}_1 \times \text{VDC}_2)$. 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.

3.3 Instruction Input

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

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

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

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

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

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

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

Table 3.1. Vector Search Code Cards

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

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

Columns

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

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

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

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

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

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

Instruction card for instructions 101 and 102:

Columns	
1–3	0 or 2 (look ahead)
4–9	101 or 102
10–18, 19–27	ORIGIN (atom number run)
28–36, 37–45	TARGET (atom number run)
46–54	*D* max (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-

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

[6]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.

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

Columns

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

3.3.3 Plotter Control Instructions (200 Series). – The 200 series is a group of instructions that control the plotter initialization, frame advance, termination, and any other peripheral commands that are required for a particular equipment configuration or plotting package. When the program is modified for a different equipment configuration, these series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements. Instructions for controlling the CalComp 580 off-line magnetic tape plotting system[7] are given here.

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

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

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

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

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

[7]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.

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

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

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

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

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

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

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

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

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

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

Columns	
1–3	Blank or 1 (depending on what follows)
4–9	401 or 411
10–18	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 number run of addressable points). The three axes of the box are parallel to the three base vectors of the reference Cartesian system, and the *semidimensions* of the box are specified on the instruction card. If an orientation of the box different from the standard orientation (see 3.1.8) is desired, than a 501 or a 502 instruction, or both, should be used before this instruction to reorient the reference Cartesian system. After this instruction has been executed, the reference system can undergo further reorientation as desired for plotting purposes, etc.

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

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

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

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

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

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

	Type A	Type B
Base vector 1 (x axis)	**u**	**u**
Base vector 2 (y axis)	**u** × **v**	(**u** × **v**) × **u**
Base vector 3 (z axis)	**u** × (**u** × **v**)	**u** × **v**

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

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

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

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

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

Columns	
	First Card
1–3	0 (or 1 if continued on next card)
4–9	502
10–18	1,2,3,−1,−2
19–27	ϕ_1°
28–36	1,2,3,−1,−2
37–45	ϕ_2°
46–54	1,2,3,−1,−2
55–63	ϕ_3°
64–72	1,2,3,−1,−2
	Second Card
10–18	ϕ_4°
.	
.	
.	

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

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

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

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

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

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

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

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

A second scale factor SCAL2 is required in connection with the ellipsoid (or sphere) size. It is a dimensionless scale factor ratio used to modify all rms displacement values before plotting 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	–	–	15.0
19–27	y_0	y_0	–	–	5.5
28–36	SCAL1	–	SCAL1	–	1.0
37–45	SCAL2	SCAL2	SCAL2	SCAL2	1.54

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

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

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

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

An ellipsoid, for graphical purposes in OR TEP, is considered to be composed of ellipses and straight lines. The ellipses are of two types, principal ellipses and boundary ellipses. Relative to the viewpoint, a principal ellipse is further subdivided into a front half and a back, or hidden, half. There are three principal ellipses per ellipsoid, corresponding to the three principal planes. The boundary ellipse is the edge of the ellipsoid as seen from the 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 3.1 shows various combinations of these elements. It is obvious that certain of these combinations are better representations than others. Instruction 701 generates the 5A model of Fig. 3.1, instruction 702 generates 2A, and 703 produces 3B. Instruction 704 draws the boundary ellipse alone. If an atom is entered as a sphere, the boundary will be circular before projection and slightly elliptical after perspective projection. Instruction 705 allows the user to make up any representation from the basic components.

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

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

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

ORNL DWG. 64-5255

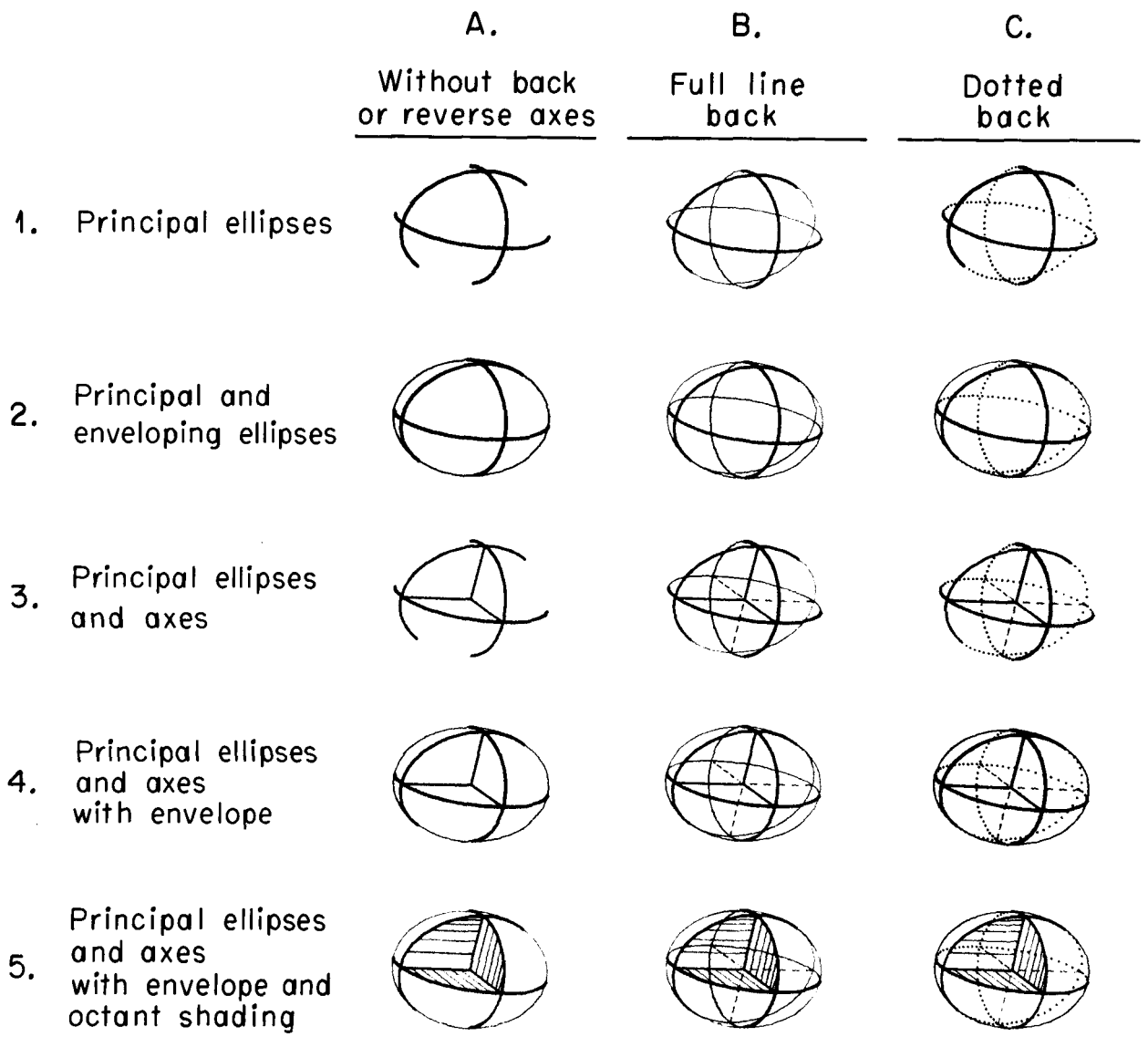

Fig. 3.1. Various Combinations of Ellipsoid Components.

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

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

where

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

A_0 is ΔR for an atom at $z = 0$, and

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

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

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

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

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

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

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

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

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

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

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

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

Second Card (needed only for boundary retracing)

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

3.3.8.2 Atom Plotting Instructions 705 and 715. –

Columns

First Card

1–3	1 (if boundary retracing is desired; otherwise 0)
4–9	705 or 715
10–18	NPLANE = 0, no ellipsoid components = 1, boundary ellipse only = 3, principal ellipses only = 4, boundary + principal ellipses
19–27	NDOT (back side of principal ellipses) <0, solid line back side = 0, back side omitted = 3, 4 dots on back side = 4, 8 dots on back side = 5, 16 dots on back side = 6, 32 dots on back side
28–36	NLINE (forward principal axes and shading) = 0, no forward axes or shading = 1, forward principal axes only = N, forward axes + (N – 1) line shading
37–45	NDASH (dashed reverse principal axes) = 0, no reverse axes = N, dashed reverse axes with N dashes
46–54	Symbol height (in.)
55–63	Perpendicular offset (in.) } for symbols
64–72	Parallel 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.[8] Each end of the bond intersects either (1) an ellipsoid or (2) an enveloping cone (tangent cone) which has its apex at the viewpoint and is tangent to an ellipsoid. In general, the ellipsoid intersection is automatically used if the axis of the bond intersects the ellipsoid at a point which is visible to the viewpoint; otherwise, the tangent cone intersection is used, so that the bond appears to terminate at the boundary of the ellipsoid. However, the user can specify that the ellipsoid intersection always be used in order to make the skeleton type model (e.g., 3B of Fig. 3.1) appear even more transparent. The radius of the stick bond and the number of lines which are used to draw the bond are specified by input parameters.

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

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

1. Bond type (for stick bond) is designated by an integer NBOND, where $-5 \leqq \text{NBOND} \leqq 5$. 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.

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.

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

3. The height of perspective labels for bond distances is entered as zero if no bond distances are to be labeled. Positive values denote the lettering height in inches before projection.

4. The perpendicular offset for bond distance perspective labels (in inches) pertains to offset of the center of the distance label relative to the center of the bond.

5. The height of regular labels for bond distances is entered as zero if no bond distances corresponding to foreshortened bonds are to be drawn. Positive values give the lettering height in inches before projection.

6. The perpendicular offset for bond-distance regular labels has the same definition as parameter 4 above.

7. The significant digits indicator is −1, 0, or 1, denoting bond distance labels with one, two, or three digits, respectively, after the decimal place.

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

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

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

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

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

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

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

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

The exact center of the label is always referred to when specifying the position of the label. The program goes through the following steps to position the center point of the label onto the drawing. (1) A point $P1$ 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 $|x \text{ edge reset}|$. No resetting is done if x *edge reset* is zero. The y parameter is handled in the same manner with y *edge reset*.

The format for the entire 900 series is as follows:

Columns	
1–3	Blank or 3 (or 1 if second card is needed)
4–9	Instruction number
10–18	Designator for atom A
19–27	Designator for atom B (or blank)
28–36	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.

3.4 List of Fault Indicators

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

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

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

Certain of the numerical 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).

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

J. Heading, *Matrix Theory for Physicists*, chap. 3, pp. 81–106, Longmans, Green and Co., London, 1958.

B. Spain, *Analytical Quadrics*, Pergamon Press, New York, 1960.

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

ORNL-DWG. 65-2671

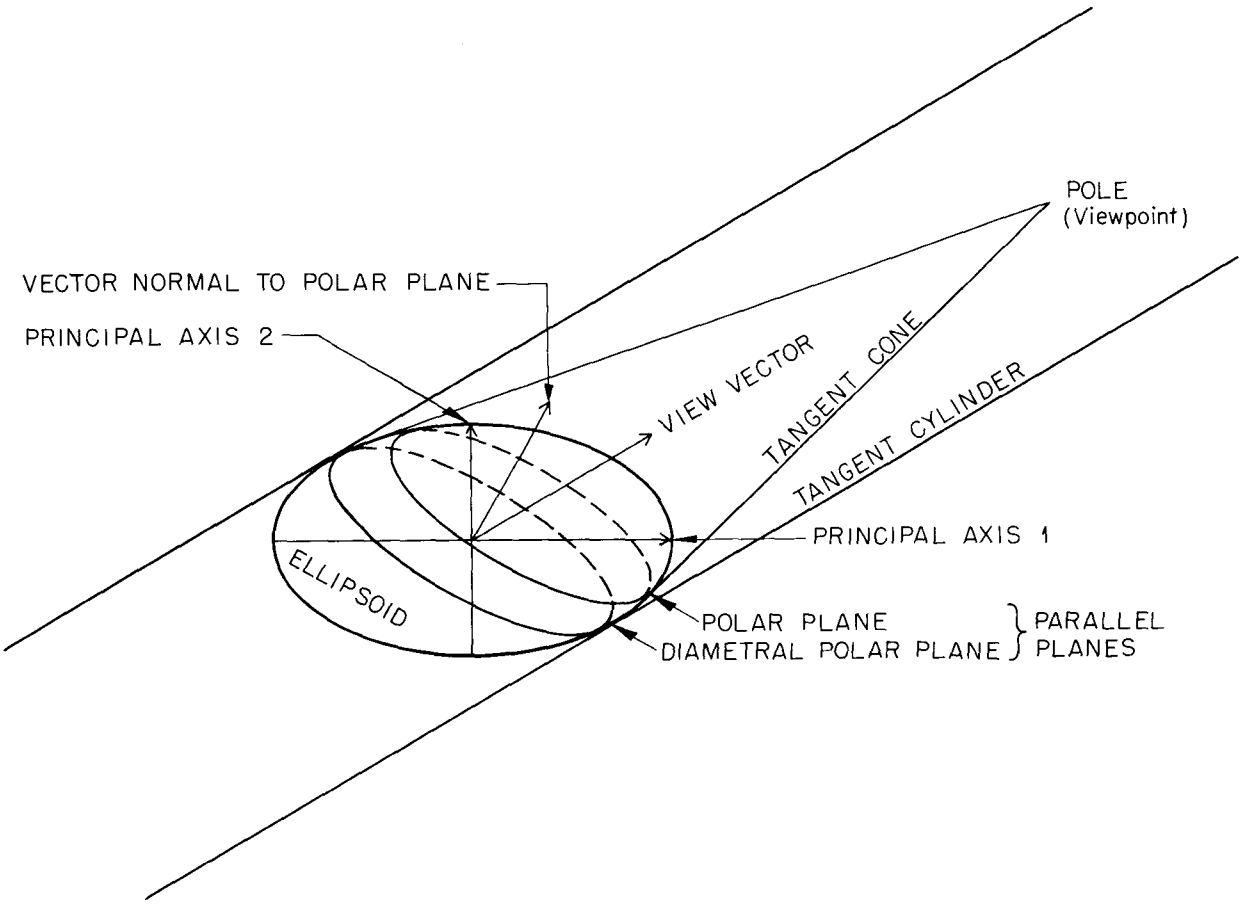

Fig. 4.1. Polar Planes Formed by Tangent Cylinder and Tangent Cone.

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

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

where i is the cycle number.

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

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

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

The ellipsoid is described in matrix notation as

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

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

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

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 **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

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

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

$$\mathbf{V}\mathbf{p} = -\mathbf{V}\mathbf{u} + \mathbf{V}\mathbf{r} ,$$

where $\mathbf{V}\mathbf{r}$ 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 = 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

4.2.3 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 **A X** = **B** for **X**. The matrices **B** and **X** are (3,N) and **A** is always (3,3). To invert **A**, make **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 **A**, each 1 A long, from the two vectors **X** and **Y**.

ITYPE > 0: Cartesian system

ITYPE ≦ 0: triclinic system

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

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

ITYPE = 0: same as type 2 except **X** = *a* crystal axis, **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 **X** − **Y** = **Z**. **Z** may have the same location as **X** or **Y**.

4.2.3.5 EIGEN (A,X,B), DIMENSION A(3,3),X(3),B(3,3). — EIGEN determines the three eigenvalues **X** and the three column eigenvectors **B** of the matrix **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 NOMBER.

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

a) ENTRY – PLOTS (A, LENGTH, LTNO)

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

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

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

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

In subroutine F200 we have

DIMENSION PLA(2000)

and card F2000170 contains

"210 CALL PLOTS (PLA,2000, LTNO)"

for the CDC 1604A or

"210 CALL PLOTS (PLA(2000),1998,LTNO)"

for the IBM 7090. The reverse storage of common in the IBM 7090 is the reason for the difference. LTNO is in common and was set to 23 by subroutine PRIME.

An ORTEP 201 instruction directs the execution of this initialization.

b) ENTRY – PLOT (X,Y,IPEN)

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

X is the abscissa expressed in inches.

Y is the ordinate expressed in inches.

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

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

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

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

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

1. The input positional parameters specified in the input argument should be an array containing *X, Y, and Z* in adjacent memory locations. Three-dimensional parameters are required to produce perspective labels. The *Z* parameter is not used by SIMBOL but is transferred to another array that is referenced when SIMBOL calls DRAW.

2. The standard routine SYMBOL calls PLOT directly while SIMBOL calls DRAW which in turn calls PLOT. When perspective labels are used, DRAW will perform a three-dimensional rotation and a projection of the grid points on which the letters are formed, to obtain true perspective. The calling sequence for DRAW is described in 4.2.2.3.

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

1. ENTRY – SIMBOL (X(1),X(2),H,BCD,THETA,N), DIMENSION X(3) (note $N \geqq 0$)

   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.

ORNL DWG. 65-2445

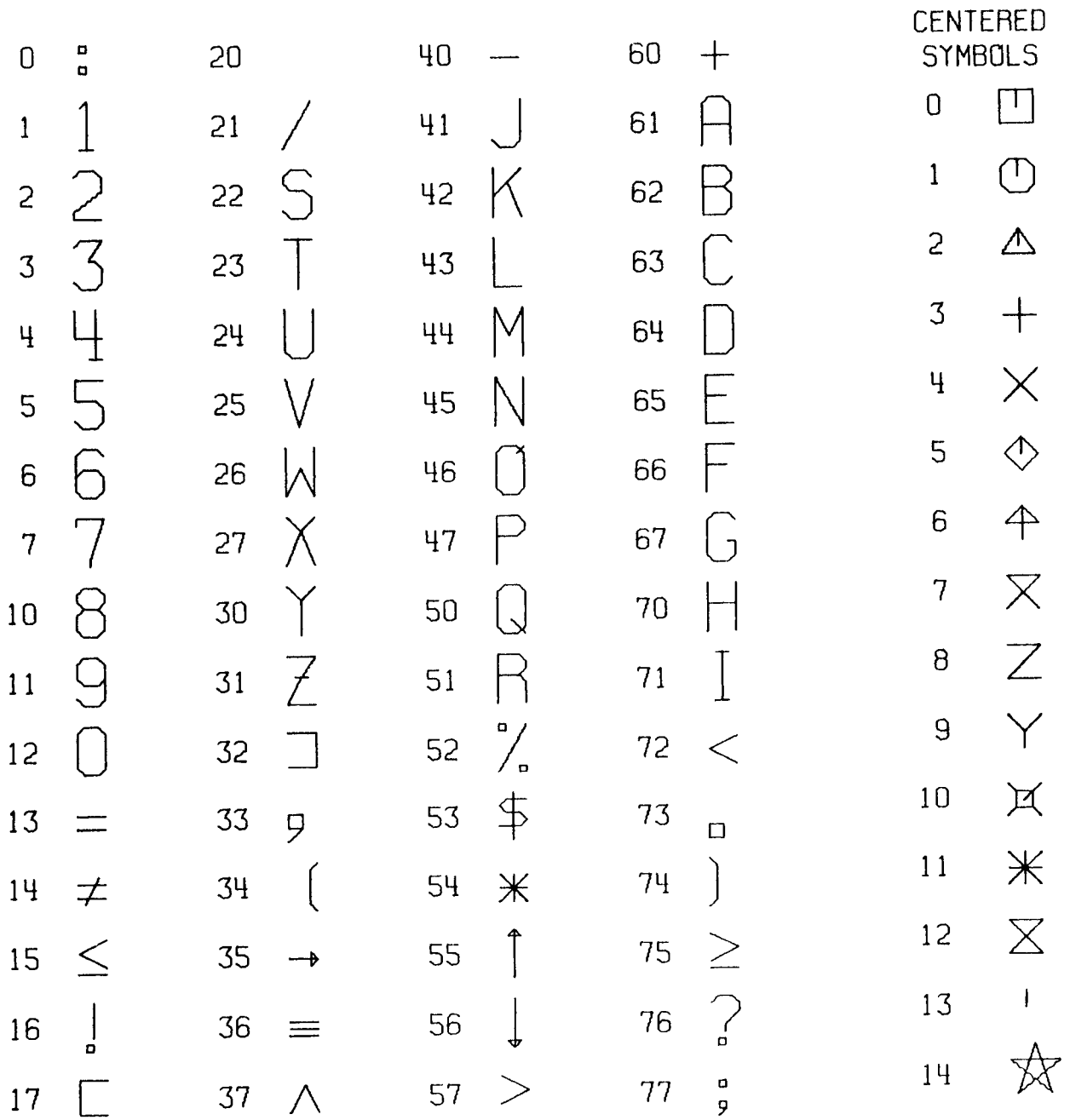

Fig. 4.2. Characters Available in 1604-A Symbol Routine.

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

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

ENTRY – NOMBER(X(1),X(2),H,A,THETA,nHFORMAT)

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

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

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

4.3 Adapting OR TEP to Other Equipment Configurations

Card decks[2] for ORTEP will be provided free of charge to crystallographers and others who request that the deck be sent to them.

The card deck contains:

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

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

1. Remove the "*LIST8" and "*LABEL" cards which precede each subprogram.
2. Place a "PROGRAM MAIN" card just before card MAIN0010.
3. Replace card F2000170 with "210 CALL PLOTS (PLA,2000,LTNO)."
4. Replace PRIM0210 with IN = 50,
   PRIM0270 with NOUT = 51,
   PRIM0280 with NSR = 57,

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

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

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

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

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

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

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

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

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

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

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

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

4.4 Addition of New OR TEP Instructions

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

The subroutines F1000 and SPARE are intended to be used for additional instructions. All 1000 series instructions call subroutine F1000, which is currently just a dummy routine. Instructions $\geqq$ 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. **BB** = $\mathbf{AA}^{-1}$.
P	BRDR	Border width in inches extending inward from plot boundary.
	CD(8,20)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(200)	Chemical symbols for the input atoms.
P	CONT(5)	Constants used in subroutine RADIAL.
	D(3,130)	Array in which three-dimensional points on an ellipse are stored by RADIAL.
	DA(3,3)	Transmits conjugate vectors to RADIAL. Also used for temporary storage.
	DP(2,130)	Array in which two-dimensional points for ellipse are stored after projection.
P	DISP	Displacement parameter for retracing.
	EDGE	Distance in inches from a projected point to the closest boundary. Set in PLTXY.
	EV(3,200)	Root-mean-square displacements for each principal axis of each input atom.
P	FORE	Cosine of critical angle between bond and Cartesian z axis vectors for perspective bond distance labels. At smaller angles the labels, produced from subroutine BOND, are drawn without perspective to prevent excessive foreshortening.
	FS(3,3,48)	Rotation matrices for input symmetry operations based on triclinic system. Used with TS array.
P	IN	Logical number for monitor input magnetic tape.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling ("Tilted Titles").
	KD(5,20)	Part of vector search code array. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
P	LTNO	Logical tape number for magnetic plotting tape.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction (vector search codes).

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

P	NG	FAULT INDICATOR (see 3.4).
	NJ	Instruction number/100.
	NJ2	Last two decimal digits of the instruction number (instruction = NJ*100 + NJ2).
P	NOUT	Logical number for monitor output magnetic tape.
P	NSR	Logical number for scratch magnetic tape.
	NSYM	Number of input symmetry operations.
	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).
	P(3,200)	Triclinic positional coordinates for the input atoms.
	PA(3,3,200)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 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 not used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.

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

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS

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

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

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 Nonsteroscopic 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.*, in press (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.*, in press (1965).

[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, *Abstracts ACA Meeting, Villanova, Pa.*, H-11 (1962).

[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 and H. A. Levy, *Abstracts ACA Meeting, Boulder, Colorado, 1961.*

[10]R. D. Ellison and H. A. Levy, *Acta Cryst.*, in press (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, *Abstracts ACA Meeting, Bozeman, Montana,* K-7 (1964) 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.*, in press (1965) and B. Morosin, private communication, 1964.

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

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

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

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

6.3 Helical Structures

OR TEP has certain features which facilitate the drawing of nonintegral helical screw models such as those discussed in the field of molecular biology. The Pauling, Corey, and Branson alpha-helix 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

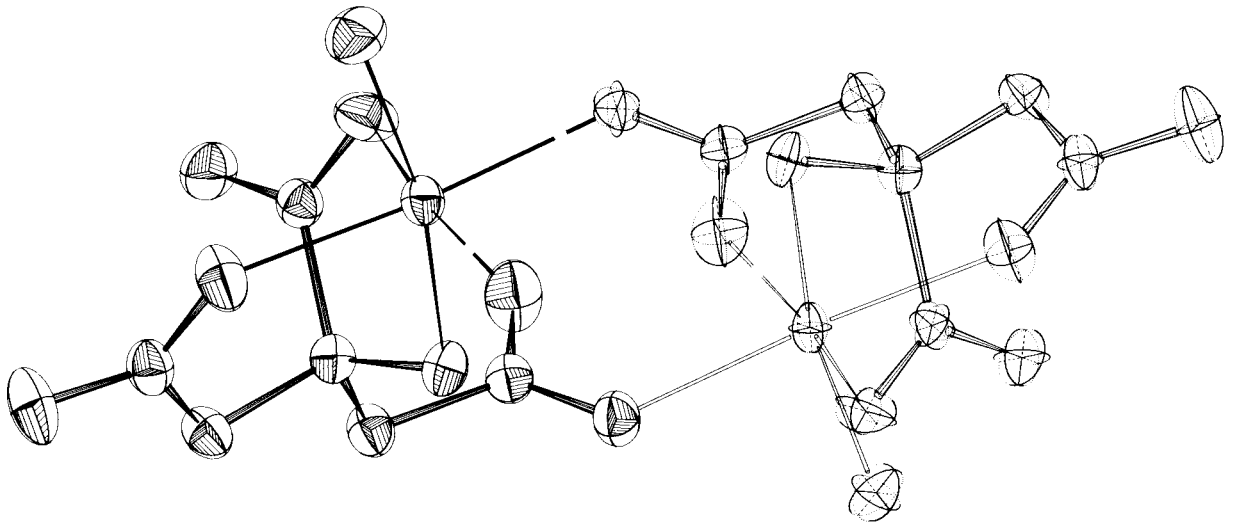

Fig. 6.1. Chelation Pattern Viewed Along a Twofold Screw Axis in the Crystal Structure of Magnesium Citrate Decahydrate. Ellipsoids represent equiprobability surfaces of thermal displacement and contain 65% of the probability distribution.

ORNL DWG. 65-2443

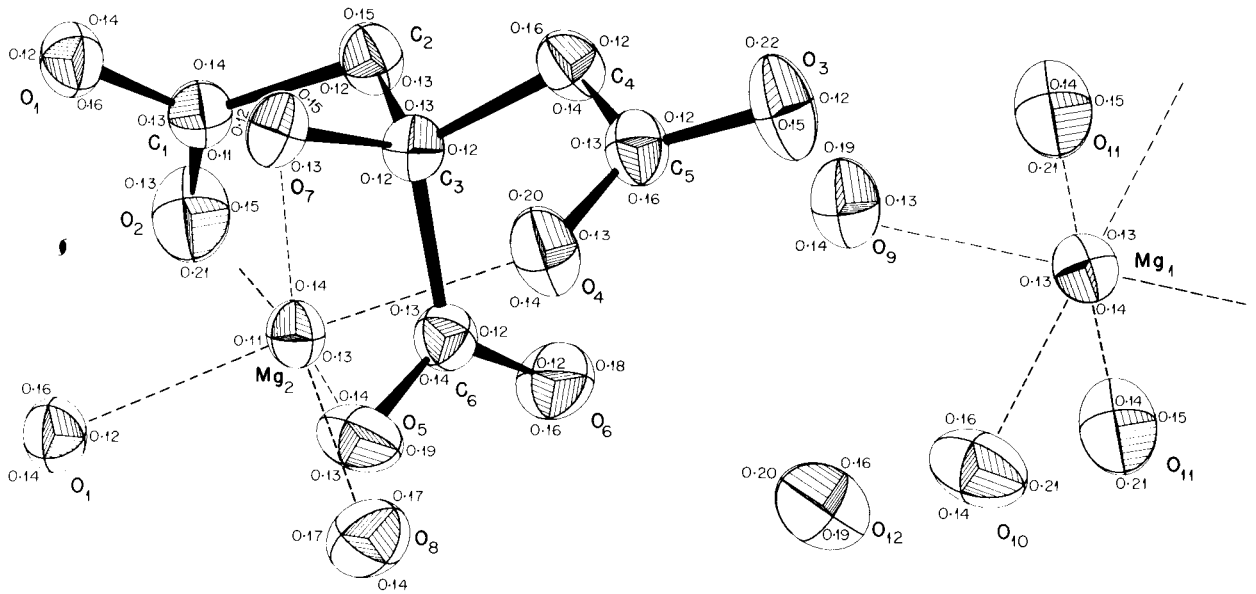

Fig. 6.2. Thermal Ellipsoid Representation for Magnesium Citrate Decahydrate with Principal Values of RMS Displacement in Angstrom Units. Ellipsoids enclose 74% probability. Structure is viewed along *b* axis.

ORNL DWG. 65-2444

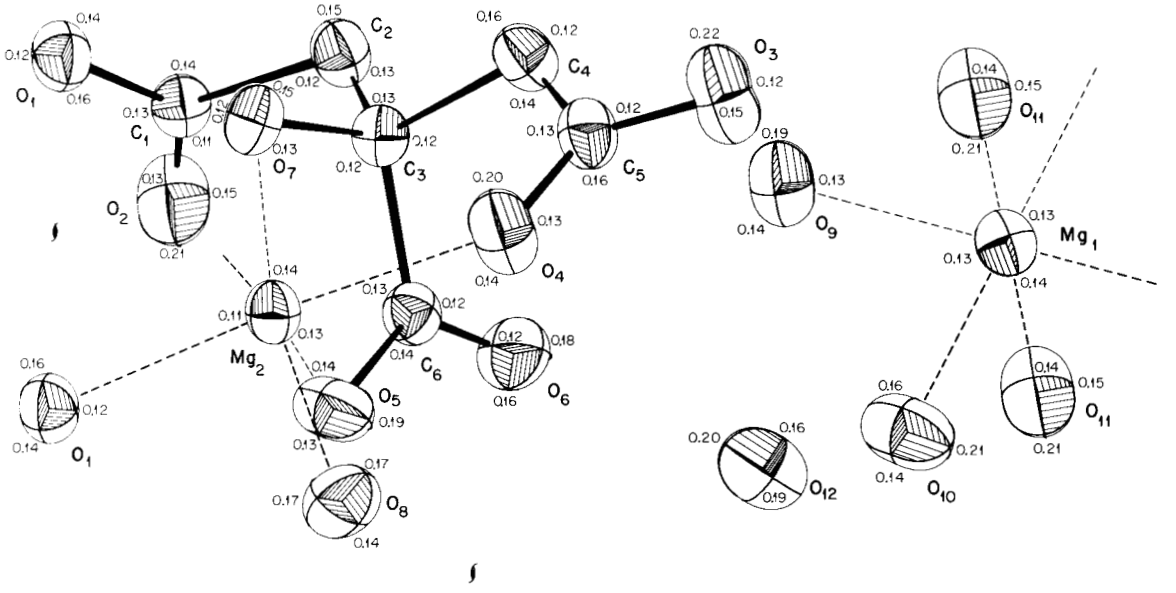

Fig. 6.3. Peanut-Shaped RMS Thermal-Displacement Figure Representation for Magnesium Citrate Decahydrate. Principal values of rms displacement in Angstrom units are indicated around the displacement figures, which are drawn at double scale. Same view of structure as shown in Fig. 6.2.

ORNL DWG. 65-2449

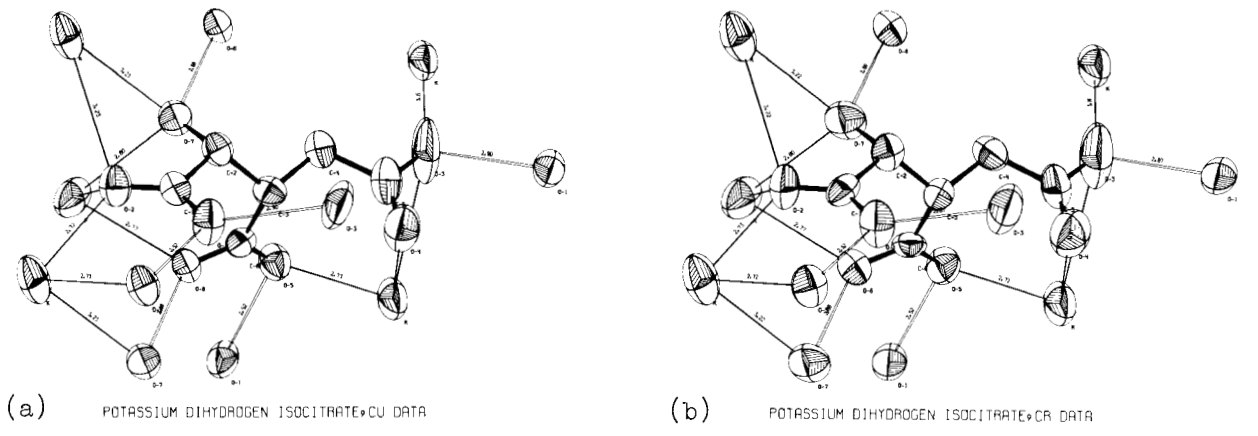

Fig. 6.4. Potassium Dihydrogen Isocitrate with Thermal Ellipsoids Scaled to Include 74% Probability. (*a*) Results obtained from 1350 three-dimensional copper K_α data (disagreement factor 6.5%). (*b*) Results obtained from 340 three-dimensional chromium K_α data (disagreement factor 2.2%). Note: This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

ORNL DWG. 65-2450

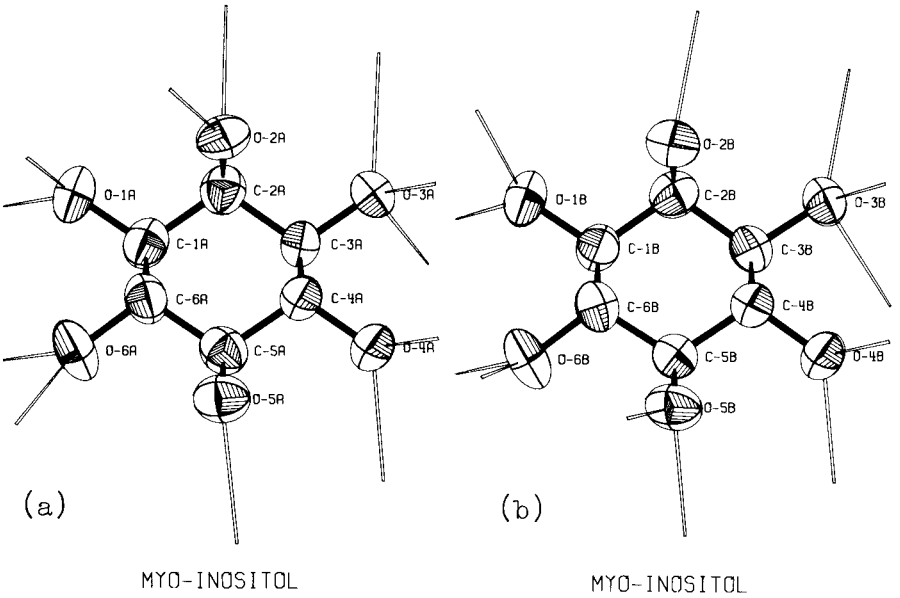

Fig. 6.5. Comparison of Thermal Ellipsoids in the Two Crystallographically Independent Molecules of Myo-Inositol (6.5*a* and 6.5*b*). Hydrogen bonding is shown, since this might influence the thermal motion. Ellipsoids are scaled to include 74% probability. Note: This is *not* a stereo pair.

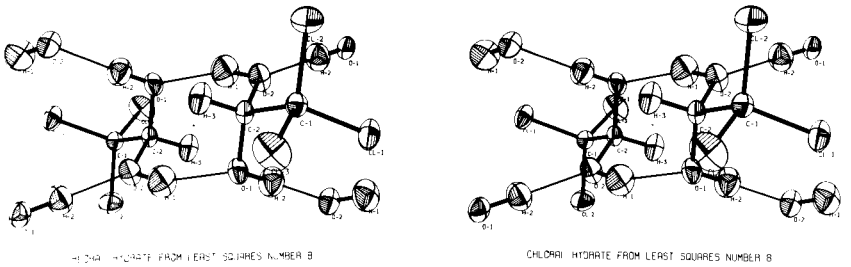

Fig. 6.6. Stereogram (Stereoscopic Pair of Perspective Projections) of Chloral Hydrate Viewed Along the Reciprocal Axis *a.** Two molecules are shown related by a center of symmetry, with the hydrogen bonds connecting them together and to other molecules. Ellipsoids are scaled to include 48% probability.

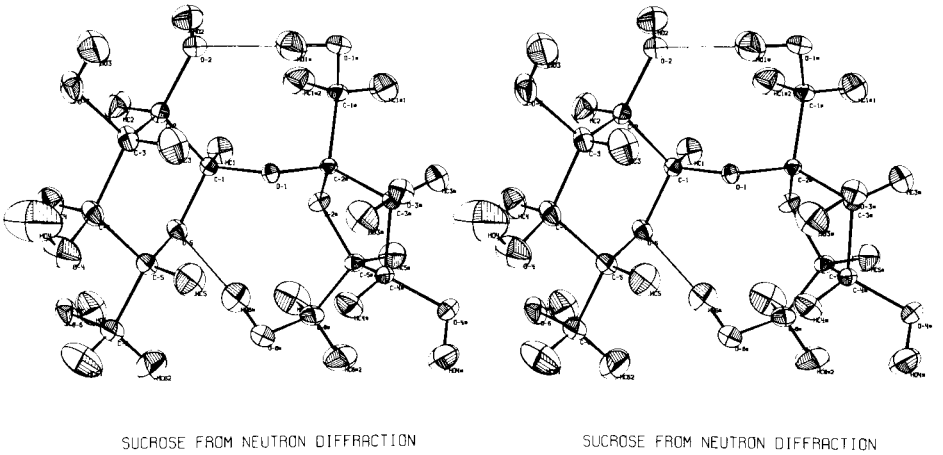

Fig. 6.7. Stereogram Showing the Sucrose Molecule with Thermal Ellipsoids Scaled to Enclose 50% Probability.

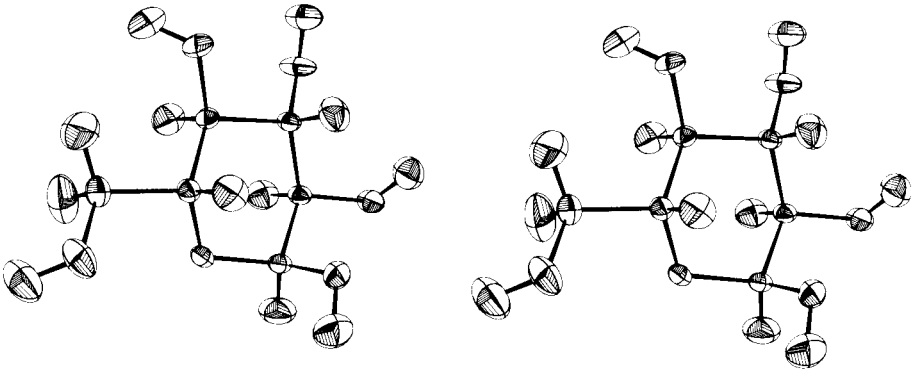

Fig. 6.8. A Molecule of Glucose with Thermal Ellipsoids Scaled to Enclose 50% Probability.

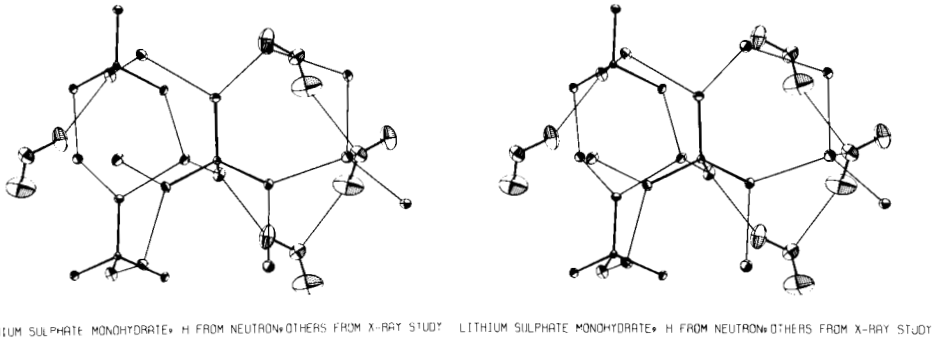

Fig. 6.9. Lithium Sulphate Monohydrate. The lithium ions and sulphate ions are coordinated into a compact network. The structure is viewed along the reciprocal a^* axis. The ellipsoids are scaled to enclose 20% probability.

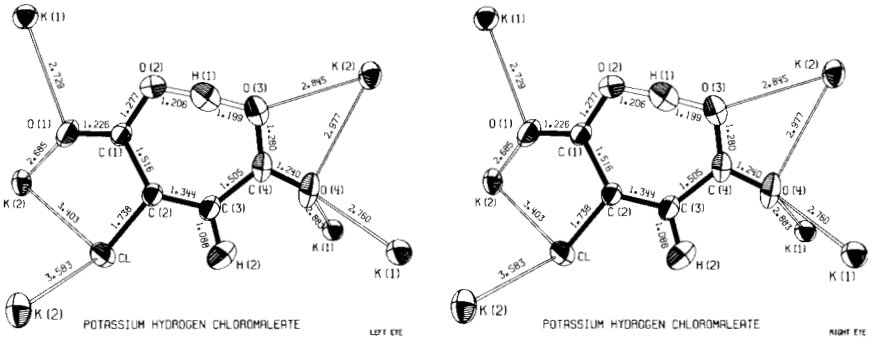

Fig. 6.10. Potassium Hydrogen Chloromaleate. The chloromaleate ion is viewed normal to its own plane. The thermal ellipsoids enclose 50% probability.

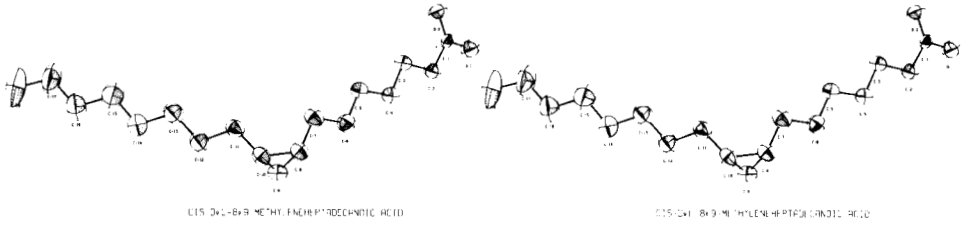

Fig. 6.11. A Molecule of Dihydromalvalic Acid with Thermal Ellipsoids Scaled to Enclose 48% Probability.

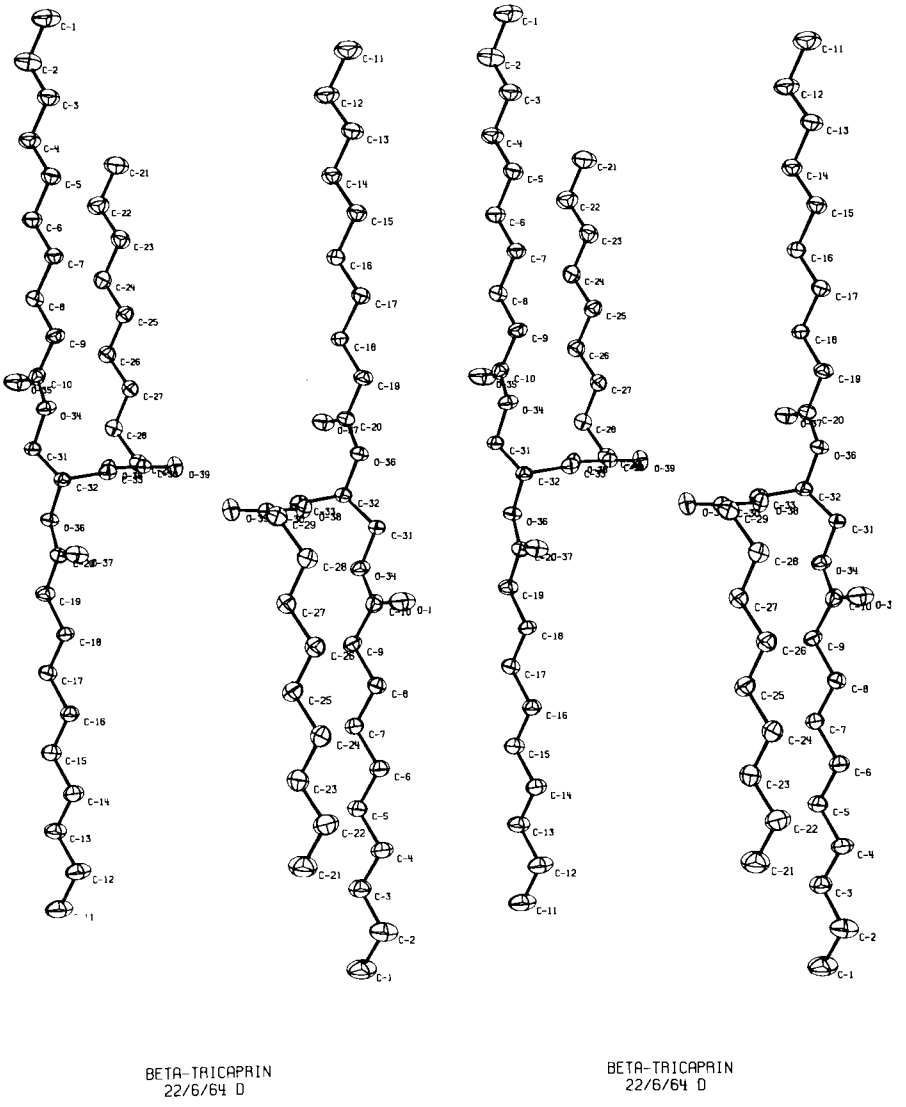

Fig. 6.12. Two Molecules of Beta-Tricaprin Related by a Center of Symmetry. The thermal ellipsoids are scaled to include 30% probability.

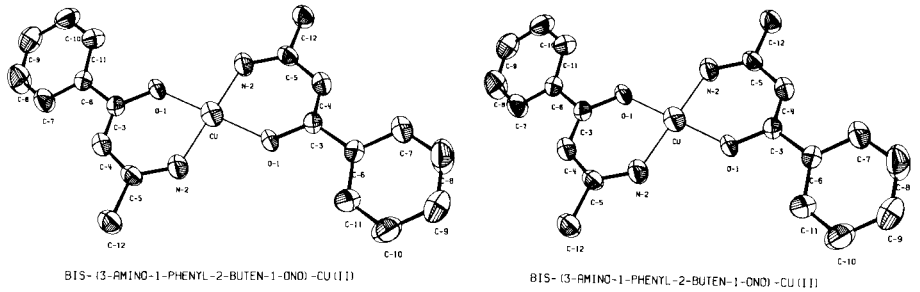

Fig. 6.13. Chelation Complex of *Bis*-(3-amino-1-phenyl-2-butene-1-ono)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

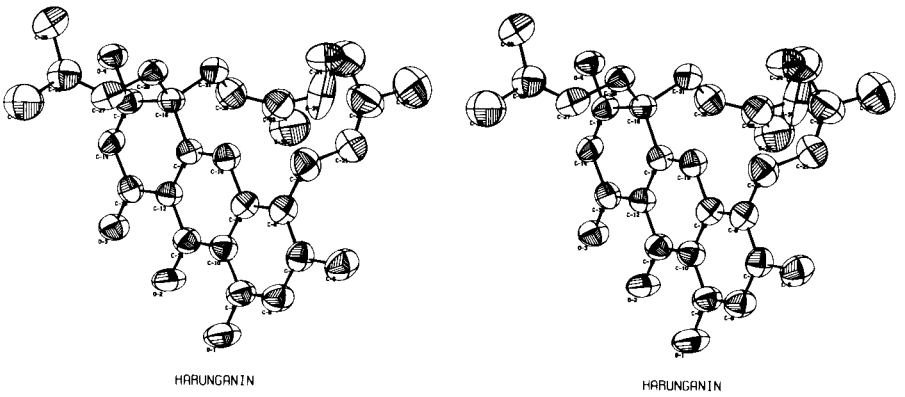

Fig. 6.14. A Molecule of the Plant Pigment Harunganin with Thermal Ellipsoids Scaled to Include 48% Probability.

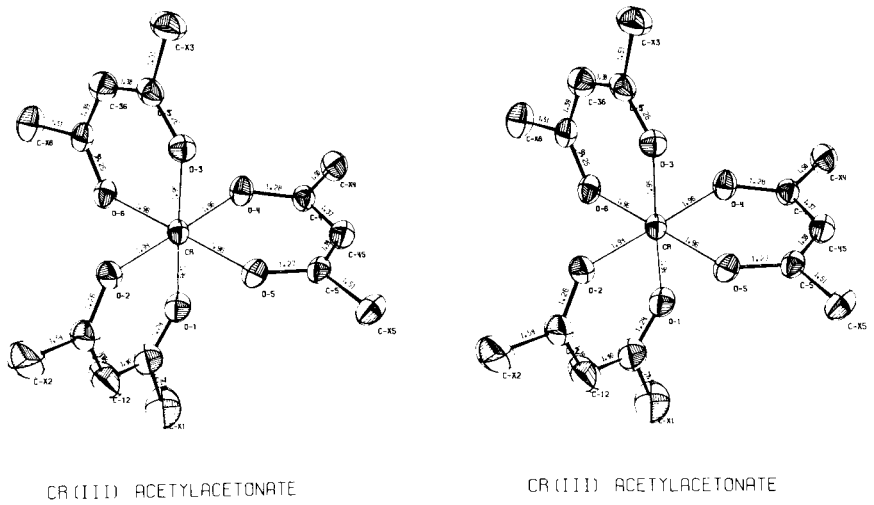

Fig. 6.15. A Unit of *Tris*-acetylacetonatochromium(III) Viewed Along its Threefold Axis of Chemical Symmetry. The thermal ellipsoids are scaled to enclose 20% probability.

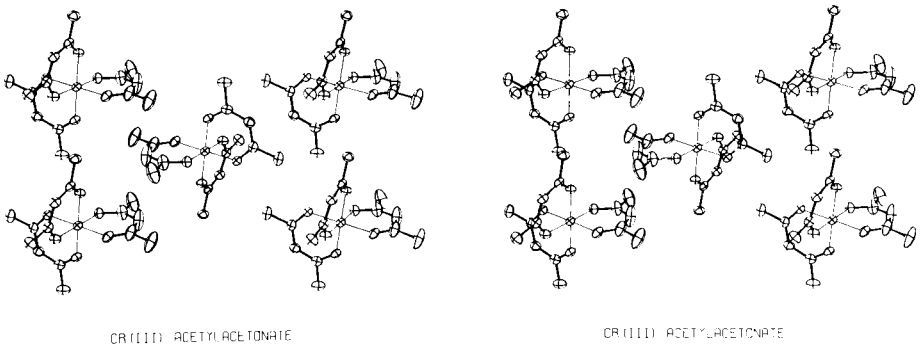

Fig. 6.16. Packing Diagrams for *Tris*-acetylacetonatochromium(III) Viewed Along the Reciprocal Axis c^*. Thermal ellipsoids are scaled to enclose 20% probability.

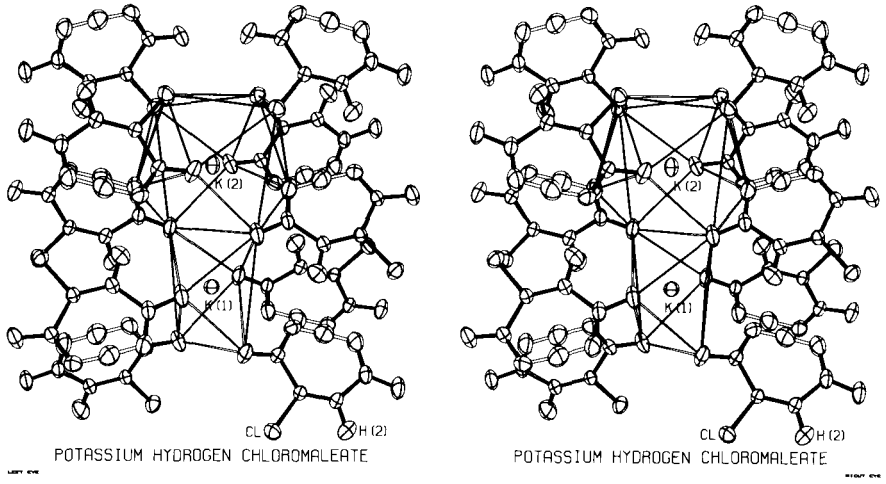

Fig. 6.17. Packing of Chloromaleate Ions Around the Potassium Ions in Potassium Hydrogen Chloromaleate. The edges of the coordination polyhedra are shown. View is nearly along the *c* axis. Thermal ellipsoids are scaled to contain 50% probability.

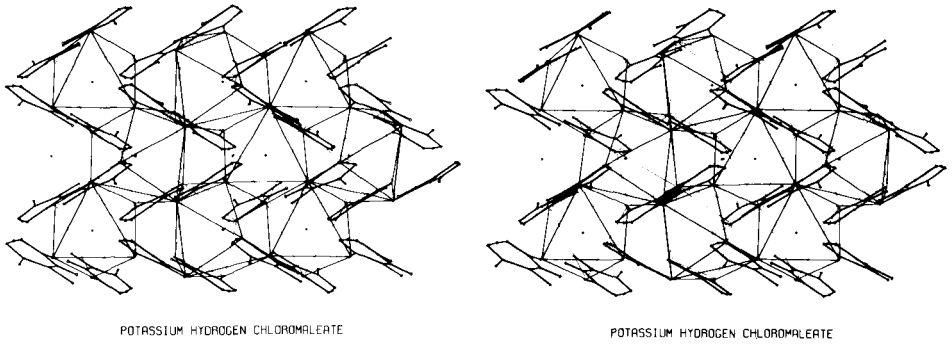

Fig. 6.18. Packing Diagrams for Potassium Hydrogen Chloromaleate. Atoms are represented as small circles. The edges of the coordination polyhedra around the potassium ions are shown. View is nearly along the *a* axis.

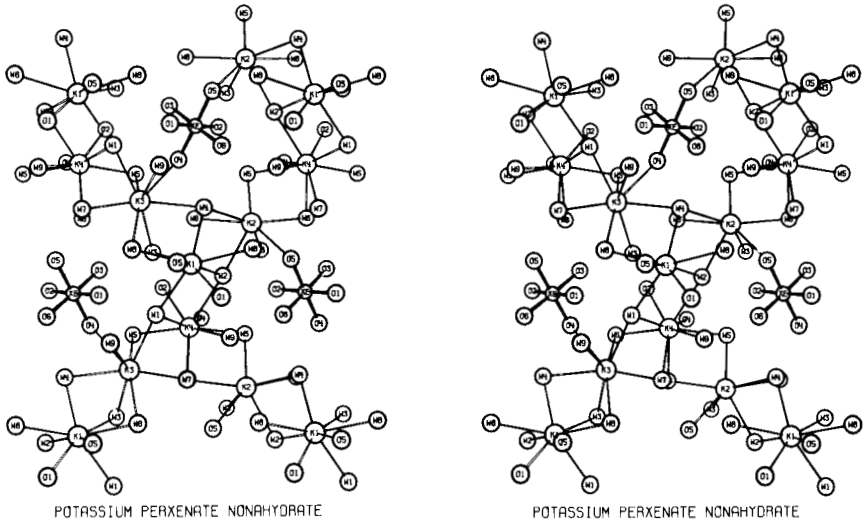

Fig. 6.19. Packing Diagram for Potassium Perxenate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Perxenate Ions. The view is parallel to the *a* axis. Another layer, related to the present one by a twofold screw axis along *a*, is needed to complete the structure.

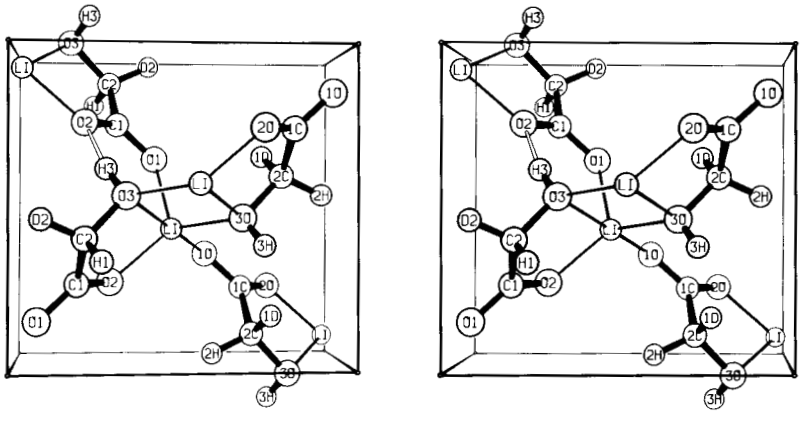

Fig. 6.20. A Stereogram Showing the Unit-Cell Contents of Anhydrous Li α-monodeuteroglycolate. The unique monoclinic *b* axis points up in the page and the mean *c* axis out from the page.

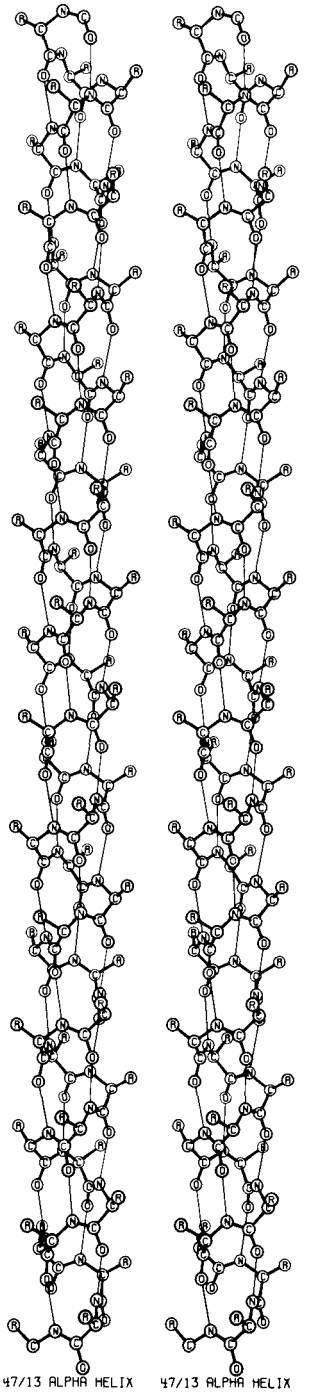

Fig. 6.21. A Stereoscopic Pair of Perspective Projections Showing the Alpha-Helix Which Is Present in Poly-L-Alanine. There are 47 amino-acid residues in 13 turns of the helix. Stereo viewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP

```
*LIST8
*LABEL
CMAIN
C       ***** OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM *****
        DIMENSICN A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)
        DIMENSICN ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)
        DIMENSICN DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3)
        DIMENSICN P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3)
        DIMENSICN RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)
        DIMENSICN VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)
        DIMENSICN XLNG(3),XO(3),XT(3)
        COMMCN NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D
        COMMCN DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD
        COMMON NJ,NJ2,NOUT,NSR,NSYM,CRGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALI
        COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2
        COMMCN V3,V4,V5,V6,WRKV,XLNG,XO,XT
      2 CALL PRIME
C       ***** READ JOB TITLE CARD *****
        READ INPUT TAPE IN,4,(TITLE(I),I#1,12)
      4 FORMAT(12A6)
        WRITE OUTPUT TAPE NOUT,6,(TITLE(I),I#1,12)
      5 FORMAT(1H010X,12A6)
      6 FORMAT(1H110X,12A6)
        CALL PRELIM
        WRITE OUTPUT TAPE NOUT,6,(TITLE(I),I#1,12)
        ISAVE#0
        GO TO 507
      7 ISAVE#0
C       ***** ZERO AIN ARRAY *****
      8 DO 10 J#1,140
     10 AIN(J)#0.
     11 FORMAT(1H04X,17H(((((( INSTRUCTIONI5,6H ))))))
     12 FORMAT(I3,I6,7F9.0)
     13 FORMAT(I3,I6,7E15.8)
     14 FORMAT(1H 9X,7E15.7)
C       ***** READ NEW INSTRUCTICN CARD *****
        NCD#0
        N1#-6
     16 N1#N1+7
        N2#N1+6
        IF(ISAVE)22,18,18
     18 READ INPUT TAPE IN,12,IC,NF,(AIN(I),I#N1,N2)
        IF(ISAVE)24,24,20
     20 WRITE OUTPUT TAPE NSR,13,IC,NF,(AIN(I),I#N1,N2)
        GO TO 24
     22 READ INPUT TAPE NSR,13,IC,NF,(AIN(I),I#N1,N2)
        IF(IC)7,24,24
     24 IF(N1-1)26,26,30
     26 WRITE OUTPUT TAPE NOUT,11,NF
        NF1#NF
        IF(NF1)28,8,30
     28 IF(NF1+2)2,2,3000
     30 WRITE OUTPUT TAPE NOUT,14,(AIN(I),I#N1,N2)
     32 IC#IC+1
        GO TO (90,16,38,50),IC
     33 FORMAT(I3,6X,5I3,8F6.0)
     34 FORMAT(6I3,8E12.5)
     35 FORMAT(1H 11X,5I3,8F11.5)
C       ***** READ FORMAT 2 TRAILER CARDS *****
     38 NCD#NCD+1
        IF(ISAVE)44,40,40
     40 READ INPUT TAPE IN,33,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)
        IF(ISAVE)46,46,42
     42 WRITE OUTPUT TAPE NSR,34,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)
        GO TO 46
     44 READ INPUT TAPE NSR,34,IC,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)
     46 WRITE OUTPUT TAPE NOUT,35,(KD(I,NCD),I#1,5),(CD(I,NCD),I#1,8)
        GO TO 32
```

```
C     ***** READ FORMAT 3 TRAILER CARD *****                          MAIN0660
   50 INN#IN                                                          MAIN0670
      IF(ISAVE)52,54,54                                               MAIN0680
   52 INN#NSR                                                         MAIN0690
   54 READ INPUT TAPE INN,4,(TITLE2(I),I#1,12)                        MAIN0700
      WRITE OUTPUT TAPE NOUT,5,(TITLE2(I),I#1,12)                     MAIN0710
      IF(ISAVE)90,90,56                                               MAIN0720
   56 WRITE OUTPUT TAPE NSR,4,(TITLE2(I),I#1,12)                      MAIN0730
C     ***** EXECUTE INSTRUCTION *****                                 MAIN0740
   90 NJ#NF1/100                                                      MAIN0750
      NJ2#NF1-NJ*100                                                  MAIN0760
      NJ3#XMODF(NJ2,10)                                               MAIN0770
      IF(NJ-12)98,92,92                                               MAIN0780
   92 CALL SPARE(NF1)                                                 MAIN0790
      IF(NG)94,8,94                                                   MAIN0800
   94 CALL ERPNT(0.,NF1)                                              MAIN0810
      GO TO 8                                                         MAIN0820
C     ******BRANCH TABLE FOR FUNCTION TYPES******                     MAIN0830
   98 GO TO(100,200,300,400,500,600,700,800,900,1000,1100),NJ         MAIN0840
C     *******STRUCTURE ANALYSIS FUNCTIONS*******                      MAIN0850
  100 GO TO (101,101,104,104,94),NJ2                                  MAIN0860
  101 CALL SEARCH                                                     MAIN0870
      GO TO 8                                                         MAIN0880
C     ***** ANISOTROPIC TEMP FACTOR OUTPUT *****                      MAIN0890
  104 DO 164 I#1,NATOM                                                MAIN0900
      IF(XMODF(I,14)-1)134,114,134                                    MAIN0910
  114 WRITE OUTPUT TAPE NOUT,6,(TITLE(J),J#1,12)                      MAIN0920
      WRITE OUTPUT TAPE NOUT,129                                      MAIN0930
  129 FORMAT(1H0 10X,4HATOM3X,16HRMS DISPLACEMENT3X,31HROW VECTORS, BASEDMAIN0940
     1 ON REFERENCE17X,29HPROBABILITY COVARIANCE MATRIX)              MAIN0950
  134 TI#55501.+FLOATF(I)*100000.                                     MAIN0960
      CALL PAXES(TI,-3)                                               MAIN0970
      IF(NG)144,154,144                                               MAIN0980
  144 CALL ERPNT(TI,104)                                              MAIN0990
  149 FORMAT(1H0 10X,A6,F10.6,6X,3F12.7,10X,3F12.7)                   MAIN1000
  154 WRITE OUTPUT TAPE NOUT,149,CHEM(I),RMS(I),(PAC(J,I),J#1,3),(Q(J,I)MAIN1010
     1,J#1,3)                                                         MAIN1020
  164 WRITE OUTPUT TAPE NOUT,159,(RMS(K),(PAC(J,K),J#1,3),(Q(J,K),J#1,3)MAIN1030
     1,K#2,3)                                                         MAIN1040
  159 FORMAT(1H 16X,F10.6,6X,3F12.7,10X,3F12.7)                       MAIN1050
      GO TO 8                                                         MAIN1060
C     *******PLOTTER INITIALIZE,FRAME ADVANCE,TERMINATE FUNCTIONS*******MAIN1070
  200 CALL F200                                                       MAIN1080
      GO TO 8                                                         MAIN1090
  300 GO TO (301,302,303,94),NJ2                                      MAIN1100
C     *******PLOT DIMENSIONS******                                    MAIN1110
  301 IF(AIN(1))321,321,311                                           MAIN1120
  311 XLNG(1)#AIN(1)                                                  MAIN1130
  321 IF(AIN(2))341,341,331                                           MAIN1140
  331 XLNG(2)#AIN(2)                                                  MAIN1150
  341 IF(AIN(3))361,361,351                                           MAIN1160
  351 VIEW#AIN(3)                                                     MAIN1170
  361 IF(AIN(4))381,381,371                                           MAIN1180
  371 BRDR#AIN(4)                                                     MAIN1190
  381 WRITE OUTPUT TAPE NOUT,389,XLNG(1),XLNG(2),BRDR                 MAIN1200
  389 FORMAT(1H0 10X,11HPLOT LIMITSF6.2,3H BYF6.2,15H IN.  INCLUDINGF6.2,MAIN1210
     112H  IN. MARGIN)                                                MAIN1220
  391 WRITE OUTPUT TAPE NOUT,399,VIEW                                 MAIN1230
  399 FORMAT(1H 10X,13HVIEW DISTANCEF7.3,7H INCHES)                   MAIN1240
      GO TO 8                                                         MAIN1250
C     *******LEGEND ROTATION*******                                   MAIN1260
  302 THETA#AIN(1)                                                    MAIN1270
      TI#THETA*.01745329252                                           MAIN1280
      COSTH#COSF(TI)                                                  MAIN1290
      SINTH#SINF(TI)                                                  MAIN1300
      DO 312 J#1,9                                                    MAIN1310
  312 SYMB(J,1)#0.                                                    MAIN1320
      SYMB(1,1)#COSTH                                                 MAIN1330
      SYMB(2,2)#COSTH                                                 MAIN1340
      SYMB(3,3)#1.                                                    MAIN1350
```

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      SYMB(2,1)#SINTH                                                   MAIN1360
      SYMB(1,2)#-SINTH                                                  MAIN1370
      WRITE OUTPUT TAPE NOUT,319,THETA                                  MAIN1380
  319 FORMAT(1H01OX,44HREGULAR TITLE AND SYMBOL ROTATION IN DEGREESF8.2)MAIN1390
      GO TO 8                                                           MAIN1400
C     ***** RETRACE DISPLACEMENT *****                                  MAIN1410
  303 DISP#AIN(1)                                                       MAIN1420
      WRITE OUTPUT TAPE NOUT,313,DISP                                   MAIN1430
  313 FORMAT(1H01OX,22HRETRACE DISPLACEMENT #F7.4,5H INCH)              MAIN1440
      GO TO 8                                                           MAIN1450
C     *******ATOM LIST FUNCTIONS******                                  MAIN1460
  400 GO TO (401,401,401,490,94,94,94,94,94,410,401,401,401,94),NJ2     MAIN1470
  401 CALL F400                                                         MAIN1480
      GO TO 490                                                         MAIN1490
  410 LATM#0                                                            MAIN1500
      DO 420 I#1,500                                                    MAIN1510
      DO 420 J#1,4                                                      MAIN1520
  420 ATCMS(J,I)#0.                                                     MAIN1530
  490 IF(LATM)8,8,491                                                   MAIN1540
  491 WRITE OUTPUT TAPE NOUT,499,(ATOMS(1,I),I#1,LATM)                  MAIN1550
  499 FORMAT(1H01OX,23HCCNTENTS OF ATOMS ARRAY/(15X,10F10.0))           MAIN1560
      GO TO 8                                                           MAIN1570
C     *******CARTESIAN COORDINATE SYSTEM FUNCTIONS*******               MAIN1580
  500 CALL F500                                                         MAIN1590
      IF(NJ3-3)507,539,539                                              MAIN1600
  507 WRITE OUTPUT TAPE NOUT,529                                        MAIN1610
      WRITE OUTPUT TAPE NOUT,519,((REFV(J,I),I#1,3),(AAREV(J,I),I#1,3),JMAIN1620
     1#1,3)                                                             MAIN1630
      GO TO 8                                                           MAIN1640
  509 FORMAT(1H01OX, 49HORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXEMAIN1650
     1S18X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VECMAIN1660
     2TOR8X,8HZ VECTOR)                                                 MAIN1670
  519 FORMAT(1H 10X,3E16.7,8X,3E16.7)                                   MAIN1680
  529 FORMAT(1H01OX,51HORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXMAIN1690
     1ES16X,33HPOST-FACTOR TRANSFORMATION MATRIX/16X,8HX VECTOR8X,8HY VEMAIN1700
     2CTOR8X,8HZ VECTOR)                                                MAIN1710
  539 WRITE OUTPUT TAPE NOUT,509                                        MAIN1720
      WRITE OUTPUT TAPE NOUT,519,((WRKV(J,I),I#1,3),(AAWRK(J,I),I#1,3),JMAIN1730
     1#1,3)                                                             MAIN1740
      GO TO 8                                                           MAIN1750
C     *******PLOT CENTERING FUNCTIONS*******                            MAIN1760
  600 CALL F600                                                         MAIN1770
      WRITE OUTPUT TAPE NOUT,609,XO(1),XO(2),SCAL1,SCAL2                MAIN1780
  609 FORMAT(1H01OX,31HORIGIN POINT IN PLOTTER COORD.(F6.2,2H ,F6.2,8H )MAIN1790
     1 IN.  / 11X,15HOVERALL SCALE #F6.3,32H INCH/ANGSTROM ELLIPSOID SCAMAIN1800
     2LE #F6.3)                                                         MAIN1810
      GO TO 391                                                         MAIN1820
C     *******ELLIPSOID AND SYMBOL PLOT FUNCTIONS*******                 MAIN1830
C     ********FILL OUT DETAILS FOR SPECIAL MODELS********               MAIN1840
  700 GO TO (701,702,704,705,709,94),NJ3                                MAIN1850
  701 AIN(3)#8.                                                         MAIN1860
      GO TO 703                                                         MAIN1870
  702 AIN(3)#0.                                                         MAIN1880
  703 AIN(1)#4.                                                         MAIN1890
      AIN(2)#0.                                                         MAIN1900
      AIN(4)#0.                                                         MAIN1910
      GO TO 709                                                         MAIN1920
  704 AIN(1)#3.                                                         MAIN1930
      AIN(2)#-5.                                                        MAIN1940
      GO TO 706                                                         MAIN1950
  705 AIN(1)#1.                                                         MAIN1960
      AIN(2)#0.                                                         MAIN1970
  706 AIN(3)#1.                                                         MAIN1980
      AIN(4)#5.                                                         MAIN1990
  709 CALL F700                                                         MAIN2000
      GO TO 8                                                           MAIN2010
C     *******8CND FUNCTIONS*******                                      MAIN2020
  800 CALL F800                                                         MAIN2030
      GO TO 8                                                           MAIN2040
C     *******TITLE FUNCTICNS*******                                     MAIN2050
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  900 CALL F900                                                         MAIN2060
      GO TO 8                                                           MAIN2070
C     *******CELL OUTLINE FUNCTIONS*******                              MAIN2080
 1000 CALL F1000                                                        MAIN2090
      GO TO 8                                                           MAIN2100
C     *******SAVE SEQUENCE FUNCTIONS*******                             MAIN2110
 1100 IF(NJ2-2)1101,1102,1103                                           MAIN2120
 1101 ISAVE#1                                                           MAIN2130
      GO TO 1104                                                        MAIN2140
 1102 ISAVE#0                                                           MAIN2150
      J#-1                                                              MAIN2160
      WRITE OUTPUT TAPE NSR,13,J,NF1,(AIN(I),I#1,7)                     MAIN2170
      END FILE NSR                                                      MAIN2180
      GO TO 1104                                                        MAIN2190
 1103 ISAVE#-1                                                          MAIN2200
 1104 REWIND NSR                                                        MAIN2210
      GO TO 8                                                           MAIN2220
 3000 CALL EXIT                                                         MAIN2230
      END                                                               MAIN2240
*LIST8
*LABEL
      FUNCTION ARCCOS(X)                                                ARCC0010
C     ARCCOS(X) IN DEGREES                                              ARCC0020
      IF(1.0-ABSF(X))1,2,2                                              ARCC0030
    1 X#SIGNF(1.0,X)                                                    ARCC0040
    2 IF(X)3,4,5                                                        ARCC0050
    3 ARCCOS#180.0+ATANF(SQRTF(1.0-X*X)/X)*57.29577951                  ARCC0060
      GO TO 6                                                           ARCC0070
    4 ARCCOS#90.0                                                       ARCC0080
      GO TO 6                                                           ARCC0090
    5 ARCCOS#ATANF(SQRTF(1.0-X*X)/X)*57.29577951                        ARCC0100
    6 RETURN                                                            ARCC0110
      END                                                               ARCC0120
*LIST8
*LABEL
      SUBROUTINE ATOM(QA,Z)                                             ATOM0010
C     ATOM COORDINATE SUBROUTINE                                        ATOM0020
      DIMENSION X(3),Z(3)                                               ATOM0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ATOM0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)ATOM0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) ATOM0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ATOM0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   ATOM0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ATOM0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     ATOM0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ATOM0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ATOM0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIATOM0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ATOM0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ATOM0150
      K#QA/100000.0                                                     ATOM0160
      IF(K)109,109,117                                                  ATOM0170
  109 X(1)#0.0                                                          ATOM0180
      X(2)#0.0                                                          ATOM0190
      X(3)#0.0                                                          ATOM0200
      GO TO 125                                                         ATOM0210
  117 IF(K-NATOM)119,119,503                                            ATOM0220
  503 NG#5                                                              ATOM0230
      GO TO 325                                                         ATOM0240
  119 DO123J#1,3                                                        ATOM0250
  123 X(J)#P(J,K)                                                       ATOM0260
  125 TA#ABSF(QA)                                                       ATOM0270
      KSYM#MODF(TA,100000.0)                                            ATOM0280
      KT#KSYM/100                                                       ATOM0290
      KS#KSYM-100*KT                                                    ATOM0300
      IF(KS-NSYM)203,203,403                                            ATOM0310
  403 NG#4                                                              ATOM0320
      GO TO 325                                                         ATOM0330
  203 IF(KS)403,205,213                                                 ATOM0340
  205 Z(1)#X(1)                                                         ATOM0350
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      Z(2)#X(2)                                                         ATOM0360
      Z(3)#X(3)                                                         ATOM0370
      GO TO 311                                                         ATOM0380
  213 DO 223 K#1,3                                                      ATOM0390
      Z(K)#TS(K,KS)                                                     ATOM0400
      DO 223 J#1,3                                                      ATOM0410
  223 Z(K)#Z(K)+FS(J,K,KS)*X(J)                                         ATOM0420
  311 IF(KT)403,325,313                                                 ATOM0430
  313 IF(KT-555)317,315,317                                             ATOM0440
  315 KSYM#KS                                                           ATOM0450
      GO TO 325                                                         ATOM0460
  317 K1#KT/100                                                         ATOM0470
      K#KT-100*K1                                                       ATOM0480
      K2#K/10                                                           ATOM0490
      K3#K-10*K2                                                        ATOM0500
      Z(1)#Z(1)+FLOATF(K1-5)                                            ATOM0510
      Z(2)#Z(2)+FLOATF(K2-5)                                            ATOM0520
      Z(3)#Z(3)+FLOATF(K3-5)                                            ATOM0530
  325 RETURN                                                            ATOM0540
      END                                                               ATOM0550
*LIST8
*LABEL
      SUBROUTINE AXEQB(A1,X,B1,JJJ)                                     AXEQ0010
C     ***** SOLUTION OF MATRIX EQUATION AX#B FOR X *****                AXEQ0020
C     ***** USES METHOD OF TRIANGULAR ELIMINATION *****                 AXEQ0030
C     ***** B AND X HAVE DIMENSIONS (3,JJJ),A IS ALWAYS (3,3)           AXEQ0040
C     ***** TO INVERT A MAKE B 3 BY 3 IDENITY MATRIX *****              AXEQ0050
      DIMENSION A1(3,3),A(3,3),B(3,3),B1(3,3),X(3,3)                    AXEQ0060
      NV#JJJ                                                            AXEQ0070
C     ***** TRANSFER DATA *****                                         AXEQ0080
      DO 2 I#1,3                                                        AXEQ0090
      DO 2 J#1,3                                                        AXEQ0100
      IF(NV-J)2,1,1                                                     AXEQ0110
    1 B(I,J)#B1(I,J)                                                    AXEQ0120
    2 A(I,J)#A1(I,J)                                                    AXEQ0130
C     ***** TRIANGULARIZE MATRIX A *****                                AXEQ0140
      DO 17 I#1,2                                                       AXEQ0150
      S#0.0                                                             AXEQ0160
      DO 4 J#I,3                                                        AXEQ0170
      R#ABSF(A(J,I))                                                    AXEQ0180
      IF(R-S)4,3,3                                                      AXEQ0190
    3 S#R                                                               AXEQ0200
      L#J                                                               AXEQ0210
    4 CONTINUE                                                          AXEQ0220
      IF(L-I)5,10,5                                                     AXEQ0230
    5 DO 6 J#I,3                                                        AXEQ0240
      S#A(I,J)                                                          AXEQ0250
      A(I,J)#A(L,J)                                                     AXEQ0260
    6 A(L,J)#S                                                          AXEQ0270
      DO 8 J#1,NV                                                       AXEQ0280
      S#B(I,J)                                                          AXEQ0290
      B(I,J)#B(L,J)                                                     AXEQ0300
    8 B(L,J)#S                                                          AXEQ0310
   10 TEM#A(I,I)                                                        AXEQ0320
      IF(TEM)11,17,11                                                   AXEQ0330
   11 IPO#I+1                                                           AXEQ0340
      DO 16 J#IPO,3                                                     AXEQ0350
      IF(A(J,I))12,16,12                                                AXEQ0360
   12 S#A(J,I)/TEM                                                      AXEQ0370
      A(J,I)#0.0                                                        AXEQ0380
      DO 13 K#IPO,3                                                     AXEQ0390
   13 A(J,K)#A(J,K)-A(I,K)*S                                            AXEQ0400
      DO 15 K#1,NV                                                      AXEQ0410
   15 B(J,K)#B(J,K)-B(I,K)*S                                            AXEQ0420
   16 CONTINUE                                                          AXEQ0430
   17 CONTINUE                                                          AXEQ0440
C     ***** MODIFY SINGULAR MATRIX *****                                AXEQ0450
      DO 20 I#1,3                                                       AXEQ0460
      IF(A(I,I))20,19,20                                                AXEQ0470
   19 A(I,I)#MAXIF(1.E-25,MAXIF(A(1,1),A(2,2),A(3,3))*1.E-15)           AXEQ0480
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   20 CONTINUE                                                          AXEQ0490
      DO 24 K#1,NV                                                      AXEQ0500
      DO 24 I#1,3                                                       AXEQ0510
      N#4-I                                                             AXEQ0520
      M#N+1                                                             AXEQ0530
      TEM#B(N,K)                                                        AXEQ0540
      IF(3-M)23,21,21                                                   AXEQ0550
   21 DO 22 J#M,3                                                       AXEQ0560
   22 TEM#TEM-A(N,J)*B(J,K)                                             AXEQ0570
   23 B(N,K)#TEM/A(N,N)                                                 AXEQ0580
   24 X(N,K)#B(N,K)                                                     AXEQ0590
      RETURN                                                            AXEQ0600
      END                                                               AXEQ0610
*LIST8
*LABEL
      SUBROUTINE AXES(U,V,X,ITYPE)                                      AXES0010
C     ***** STORE THREE ORTHOGONAL VECTORS EACH 1 ANGSTROM LONG *****   AXES0020
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         AXES0030
C     ***** XABSF(ITYPE)#1 W(1)#U,W(2)#(UXV),W(3)#UX(UXV) *****         AXES0040
C     ***** XABSF(ITYPE)#2 W(1)#U,W(2)#(UXV)XU,W(3)#(UXV) *****         AXES0050
C     ***** ITYPE#0 W(1)#A,W(2)#(AXB)XA,W(3)#(AXB), ABC#CELL VECTORS ***AXES0060
      DIMENSION U(3),V(3),W(3,3),X(3,3)                                 AXES0070
      IT#ITYPE                                                          AXES0080
      IF(IT)115,105,115                                                 AXES0090
  105 U(1)#1.                                                           AXES0100
      U(2)#0.                                                           AXES0110
      U(3)#0.                                                           AXES0120
      V(1)#0.                                                           AXES0130
      V(2)#1.                                                           AXES0140
      V(3)#0.                                                           AXES0150
  115 DO 125 J#1,3                                                      AXES0160
  125 W(J,1)#U(J)                                                       AXES0170
      IF(XABSF(IT)-1)145,135,145                                        AXES0180
  135 CALL NORM(U,V,W(1,2),IT)                                          AXES0190
      CALL NORM(U,W(1,2),W(1,3),IT)                                     AXES0200
      GO TO 155                                                         AXES0210
  145 CALL NORM(U,V,W(1,3),IT)                                          AXES0220
      CALL NORM(W(1,3),U,W(1,2),IT)                                     AXES0230
  155 DO 195 I#1,3                                                      AXES0240
      IF(IT)165,165,175                                                 AXES0250
  165 IC#-1                                                             AXES0260
      GO TO 195                                                         AXES0270
  175 IC#1                                                              AXES0280
  195 CALL UNIT(W(1,I),X(1,I),IC)                                       AXES0290
      RETURN                                                            AXES0300
      END                                                               AXES0310
*LIST8
*LABEL
      SUBROUTINE BOND(Z1,Z2,NB)                                         BOND0010
      DIMENSION B(3,3),E(3,3),R(3,3),RT(3,3),S(3,3),U(3,3),VUE(3)       BOND0020
      DIMENSION V7(3),W(13,2),X(3),Z(3)                                 BOND0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    BOND0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)BOND0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) BOND0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) BOND0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   BOND0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   BOND0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     BOND0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   BOND0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATN,LTNO,NATOM,NCD BOND0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIBOND0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   BOND0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                BOND0150
C     ***** OBTAIN POSITIONAL PARAMETERS *****                          BOND0160
      NG1#0                                                             BOND0170
      DO 105 J#1,26                                                     BOND0180
  105 W(J,1)#0.                                                         BOND0190
      W(1,1)#Z1                                                         BOND0200
      W(1,2)#Z2                                                         BOND0210
      DO 135 I#1,2                                                      BOND0220
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      CALL XYZ(W(1,I),W(4,I),2)                                         BOND0230
      IF(NG)125,110,125                                                 BOND0240
  110 DO 115 J#1,3                                                      BOND0250
  115 W(J+6,I)#XT(J)                                                    BOND0260
      K#W(1,I)/100000.                                                  BOND0270
      L#W(1,I)-FLOATF(K)*100000.                                        BOND0280
      CALL PLTXY(W(4,I),W(2,I))                                         BOND0290
      IF(EDGE-BRDR*.25)120,128,128                                      BOND0300
  120 NG#10                                                             BOND0310
  125 NGI#1                                                             BOND0320
      WRITE OUTPUT TAPE NOUT,136,CHEM(K),K,L,(W(J,I),J#2,9)             BOND0330
      CALL ERPNT(W(1,I),800)                                            BOND0340
      GO TO 135                                                         BOND0350
  128 IF(NJ2-10)130,135,135                                             BOND0360
  130 WRITE OUTPUT TAPE NOUT,136,CHEM(K),K,L,(W(J,I),J#2,9)             BOND0370
  135 CONTINUE                                                          BOND0380
  136 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)   2F8.2,5X,3F8.3,13X,3F8.4)    BOND0390
      IF(NGI)999,140,999                                                BOND0400
  140 CALL DIFV(W(7,1),W(7,2),V7)                                       BOND0410
      DIST#SQRTF(VMV(V7,AA,V7))                                         BOND0420
      IF(XMODF(NJ2,10)-3)143,142,142                                    BOND0430
  142 HGT#SCAL1*.12                                                     BOND0440
      CALL SIMBOL(W(2,1),W(3,1),HGT,XMODF(XFIXF(W(1,1)/100000.),10),0.,-BOND0450
     11)                                                                BOND0460
      CALL SIMBOL(W(2,2),W(3,2),HGT,XMODF(XFIXF(W(1,2)/100000.),10),0.,-BOND0470
     12)                                                                BOND0480
      GO TO 570                                                         BOND0490
  143 KODE#KD(5,NB)                                                     BOND0500
      IF(KODE)145,144,146                                               BOND0510
  144 NBND#0                                                            BOND0520
      GO TO 148                                                         BOND0530
  145 KODE#-KODE                                                        BOND0540
  146 NBND#128/2**KODE                                                  BOND0550
C     ***** FIND UPPERMOST ATOM PUT IN POSITION ONE *****               BOND0560
  148 IF(VIEW)152,150,152                                               BOND0570
  150 W(12,1)#1.                                                        BOND0580
      W(12,2)#1.                                                        BOND0590
      IF(W(6,1)-W(6,2))165,175,175                                      BOND0600
C     *****VECTOR FROM ATOM TO VIEWPOINT *****                          BOND0610
  152 DO 160 I#1,2                                                      BOND0620
      DO 155 J#10,12                                                    BOND0630
  155 W(J,I)#-W(J-6,I)                                                  BOND0640
      W(12,I)#W(12,I)+VIEW                                              BOND0650
C     ***** DISTANCE SQUARED TO VIEWPOINT *****                         BOND0660
  160 W(13,I)#VV(W(10,I),W(10,I))                                       BOND0670
      IF(W(13,2)-W(13,1))165,175,175                                    BOND0680
C     ***** SWITCH ATOMS *****                                          BOND0690
  165 DO 170 J#1,13                                                     BOND0700
      TI#W(J,1)                                                         BOND0710
      W(J,1)#W(J,2)                                                     BOND0720
  170 W(J,2)#TI                                                         BOND0730
C     ***** FORM IDEMFACTOR MATRIX *****                                BOND0740
  175 DO 180 J#1,3                                                      BOND0750
      E(J,J)#1.                                                         BOND0760
      E(J+1,1)#0.                                                       BOND0770
  180 E(J+5,1)#0.                                                       BOND0780
C     ***** FORM VECTOR SET RADIAL TO BOND *****                        BOND0790
      CALL DIFV(W(4,2),W(4,1),DA(1,3))                                  BOND0800
      CALL UNIT(DA(1,3),V3,1)                                           BOND0810
      T6#ABSF(V3(3))                                                    BOND0820
      IF(.9994-T6)390,185,185                                           BOND0830
  185 TI#CD(3,NB)/SCAL2                                                 BOND0840
      CALL AXES(V3,E(1,3),B,1)                                          BOND0850
      DO 190 J#1,3                                                      BOND0860
      DA(J,1)#-B(J,2)*TI                                                BOND0870
  190 DA(J,2)#-B(J,3)*TI                                                BOND0880
      IF(NBND)500,500,195                                               BOND0890
  195 CALL RADIAL(3)                                                    BOND0900
C     ***** DERIVE QUADRICS FOR EACH ATOM *****                         BOND0910
      DO 380 II#1,2                                                     BOND0920
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      CALL PAXES(W(1,II),2)                                             BOND0930
      IF(NG)205,210,205                                                 BOND0940
  205 CALL ERPNT(W(1,II),800)                                           BOND0950
      GO TO 999                                                         BOND0960
C     ***** DOES BOND GO TO ELLIPSOID OR TO ENVELOPE *****              BOND0970
  210 T1#3-II*2                                                         BOND0980
      DO 212 J#1,3                                                      BOND0990
      V3(J)#V3(J)*T1                                                    BOND1000
  212 VUE(J)#0.                                                         BOND1010
      IF(KD(5,NB))260,260,215                                           BOND1020
  215 CALL UNIT(W(10,II),R(1,3),1)                                      BOND1030
      IF(VMV(V3,Q,R(1,3)))220,260,260                                   BOND1040
C     ***** ESTABLISH VIEW COORDINATE SYSTEM *****                      BOND1050
  220 IBND#0                                                            BOND1060
      IF(VIEW)225,225,230                                               BOND1070
C     ***** DERIVE TANGENT CYLINDER *****                               BOND1080
  225 CONE#0.                                                           BOND1090
      GO TO 240                                                         BOND1100
C     ***** DERIVE TANGENT CONE *****                                   BOND1110
  230 CONE#SCL*SCL/W(13,II)                                             BOND1120
      CALL NORM(E(1,2),R(1,3),R(1,1),1)                                 BOND1130
      CALL UNIT(R(1,1),R(1,1),1)                                        BOND1140
      CALL NORM(R(1,3),R(1,1),R(1,2),1)                                 BOND1150
      DO 235 I#1,3                                                      BOND1160
      DO 235 J#1,3                                                      BOND1170
  235 RT(I,J)#R(J,I)                                                    BOND1180
C     ***** BASE ELLIPSOID ON VIEW COORDINATE SYSTEM *****              BOND1190
      CALL MM(RT,Q,U)                                                   BOND1200
      CALL MM(U,R,Q)                                                    BOND1210
  240 T1#1./(CONE-Q(3,3))                                               BOND1220
      T2#CONE*T1                                                        BOND1230
      DO 250 J#1,2                                                      BOND1240
      DO 245 K#1,2                                                      BOND1250
  245 S(K,J)#Q(K,J)+Q(K,3)*Q(J,3)*T1                                    BOND1260
      S(3,J)#Q(3,J)*T2                                                  BOND1270
  250 S(J,3)#Q(J,3)*T2                                                  BOND1280
      S(3,3)#Q(3,3)*T2                                                  BOND1290
      IF(CONE)252,270,252                                               BOND1300
  252 DO 255 J#1,3                                                      BOND1310
  255 VUE(J)#-W(J+9,II)/SCL                                             BOND1320
C     ***** BASE TANGENT CONE ON WORKING SYSTEM *****                   BOND1330
      CALL MM(R,S,U)                                                    BOND1340
      CALL MM(U,RT,S)                                                   BOND1350
      T5#0.                                                             BOND1360
      GO TO 300                                                         BOND1370
C     ***** TRANSFER ELLIPSOID *****                                    BOND1380
  260 DO 265 J#1,9                                                      BOND1390
  265 S(J,1)#Q(J,1)                                                     BOND1400
      IBND#II                                                           BOND1410
  270 T5#1.                                                             BOND1420
C     ***** CHECK FOR BOND TAPER *****                                  BOND1430
  300 IF(II-2)305,310,310                                               BOND1440
  305 RADIUS#1.+T6*TAPER                                                BOND1450
      GO TO 320                                                         BOND1460
  310 RADIUS#1.-T6*TAPER                                                BOND1470
  320 CALL MV(S,V3,V4)                                                  BOND1480
      T2#VV(V3,V4)                                                      BOND1490
C     ***** COMPUTE BOND INTERSECTION *****                             BOND1500
      KL#5-II-II                                                        BOND1510
      DO 360 K#1,65,4                                                   BOND1520
      DO 325 J#1,3                                                      BOND1530
      V6(J)#D(J,K)*RADIUS                                               BOND1540
  325 V5(J)#V6(J)+VUE(J)                                                BOND1550
      T3#VV(V5,V4)                                                      BOND1560
      T4#T3*T3-T2*(VMV(V5,S,V5)-T5)                                     BOND1570
      IF(T4)330,335,335                                                 BOND1580
  330 NG#13                                                             BOND1590
      CALL ERPNT(W(1,II),800)                                           BOND1600
      GO TO 999                                                         BOND1610
  335 T4#SQRTF(T4)                                                      BOND1620
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      T1#(T4-T3)/T2                                                     BOND1630
      T3#(-T4-T3)/T2                                                    BOND1640
      L#K+KL-1                                                          BOND1650
      DO 360 J#1,3                                                      BOND1660
      D(J,L)#(V6(J)+T1*V3(J))*SCL                                       BOND1670
  360 D(J,L+1)#(-V6(J)-T3*V3(J))*SCL                                    BOND1680
      CALL PRCJ(D(1,KL)  ,DP(1,II),W(4,II),XO,VIEW,1,65,4)              BOND1690
      IF(IBND-1)370,365,370                                             BOND1700
  365 CALL PRCJ(D(1,KL+5),DP(1,II+68),W(4,II),XO,VIEW,1,61,4)           BOND1710
      GO TO 380                                                         BOND1720
C     ***** RETRACE TOP HALF *****                                      BOND1730
  370 DO 375 K#4,64,4                                                   BOND1740
      L#K+II                                                            BOND1750
      M#L+64                                                            BOND1760
      N#66-L                                                            BOND1770
      DP(1,M)#DP(1,N)                                                   BOND1780
  375 DP(2,M)#DP(2,N)                                                   BOND1790
  380 CONTINUE                                                          BOND1800
C     ***** CHECK FOR OVERLAP OR HIDDEN BOND *****                      BOND1810
      DO 395 K#1,65,32                                                  BOND1820
      T1#0.                                                             BOND1830
      T2#0.                                                             BOND1840
      DO 385 J#1,2                                                      BOND1850
      T1#T1+(DP(J,K)-W(J+1,1))**2                                       BOND1860
  385 T2#T2+(DP(J,K+1)-W(J+1,1))**2                                     BOND1870
      IF(T2-T1)390,390,395                                              BOND1880
  390 NG#14                                                             BOND1890
      CALL ERPNT(W(1,2),800)                                            BOND1900
      GO TO 999                                                         BOND1910
  395 CCNTINUE                                                          BOND1920
C     ***** DRAW BCND OUTLINE *****                                     BOND1930
      CALL DRAW(DP(1,1),0.,0.,3)                                        BOND1940
      DO 415 K#5,129,4                                                  BOND1950
  415 CALL DRAW(DP(1,K),0.,0.,2)                                        BOND1960
      DO 420 K#2,66,4                                                   BOND1970
  420 CALL DRAW(DP(1,K),0.,0.,2)                                        BOND1980
      CALL DRAW(DP(1,65),0.,0.,2)                                       BOND1990
C     ***** DRAW BCND DETAIL *****                                      BOND2000
  425 K#65                                                              BOND2010
  430 K#K-NBND                                                          BOND2020
      IF(K-1)500,500,435                                                BOND2030
  435 CALL DRAW(DP(1,K),0.,0.,3)                                        BOND2040
      CALL DRAW(DP(1,K+1),0.,0.,2)                                      BOND2050
      K#K-NBND                                                          BOND2060
      IF(K-1)500,500,440                                                BOND2070
  440 CALL DRAW(DP(1,K+1),0.,0.,3)                                      BOND2080
      CALL DRAW(DP(1,K),0.,0.,2)                                        BOND2090
      GO TO 430                                                         BOND2100
  500 HGT#CD(4,NB)                                                      BOND2110
      OFF#CD(5,NB)                                                      BOND2120
      IF(HGT)510,570,510                                                BOND2130
C     ***** PERSPECTIVE BCND LABEL ROUTINE *****                        BOND2140
C     ***** BASE DECISICNS ON REFERENCE SYSTEM *****                    BOND2150
  510 K#0                                                               BOND2160
      CALL DIFV(W(7,2),W(7,1),V7)                                       BOND2165
      CALL VM(V7,AAREV,V1)                                              BOND2170
      CALL AXES(V1,E(1,3),U,1)                                          BOND2180
      DO 535 I#1,3                                                      BOND2190
      T1#1.                                                             BOND2200
      IF(I-2)515,515,520                                                BOND2210
  515 IF(VV(U(1,I),SYMB(1,I)))525,530,530                               BOND2220
  520 IF(XMODF(K,2))530,525,530                                         BOND2230
  525 T1#-1.                                                            BOND2240
      K#K+1                                                             BOND2250
  530 DO 535 J#1,3                                                      BOND2260
      U(J,I)#U(J,I)*T1                                                  BOND2270
  535 VT(J,I)#B(J,I)*T1                                                 BOND2280
      DO 540 J#1,3                                                      BOND2290
  540 VT(J,4)#.5*(W(J+3,1)+W(J+3,2))                                    BOND2300
C     ***** CHECK FOR EXCESS FORESHORTENING *****                       BOND2310
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      IF(FORE-ABSF(U(3,1)))545,550,550                                  BOND2320
  545 CALL NORM(U(1,2),SYMB(1,3),VT(1,1),1)                             BOND2330
      VT(1,3)#SYMB(1,3)                                                 BOND2340
      VT(2,3)#SYMB(2,3)                                                 BOND2350
      VT(3,3)#SYMB(3,3)                                                 BOND2360
      HGT#CD(6,NB)                                                      BOND2370
      OFF#CD(7,NB)                                                      BOND2380
      IF(HGT)550,999,550                                                BOND2390
  550 TI#CD(8,NB)                                                       BOND2400
      Z(1)#VT(1,4)-HGT*(23.-3.*TI)/7.                                   BOND2410
      Z(2)#VT(2,4)+OFF-HGT*.5                                           BOND2420
      Z(3)#VT(3,4)                                                      BOND2430
      ITILT#1                                                           BOND2440
      IF(TI)555,560,565                                                 BOND2450
  555 CALL NOMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.1)                         BOND2460
      GO TO 570                                                         BOND2470
  560 CALL NOMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.2)                         BOND2480
      GO TO 570                                                         BOND2490
  565 CALL NOMBER(Z(1),Z(2),HGT,DIST,0.,4HF6.3)                         BOND2500
  570 ITILT#0                                                           BOND2510
      IF(NJ2-10)580,999,999                                             BOND2520
  580 WRITE OUTPUT TAPE NOUT,571,DIST                                   BOND2530
  571 FORMAT(1H 59X,10HDISTANCE #F8.3/1H )                              BOND2540
  999 RETURN                                                            BOND2550
      END                                                               BOND2560
*LIST8
*LABEL
      SUBROUTINE DIFV(X,Y,Z)                                            DIFV0010
C     VECTOR - VECTOR                                                   DIFV0020
C     Z(3)#X(3)-Y(3)                                                    DIFV0030
      DIMENSIONX(3),Y(3),Z(3)                                           DIFV0040
      DO111I#1,3                                                        DIFV0050
  111 Z(I)#X(I)-Y(I)                                                    DIFV0060
      RETURN                                                            DIFV0070
      END                                                               DIFV0080
*LIST8
*LABEL
      SUBROUTINE DRAW(W,DX,DY,NPEN)                                     DRAW0010
      DIMENSION W(3),X(3),Y(3),Z(3)                                     DRAW0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    DRAW0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)DRAW0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) DRAW0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) DRAW0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   DRAW0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   DRAW0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     DRAW0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   DRAW0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD DRAW0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIDRAW0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   DRAW0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                DRAW0140
      Y(1)#W(1)+DX                                                      DRAW0150
      Y(2)#W(2)+DY                                                      DRAW0160
      IF(ITILT)115,140,115                                              DRAW0170
C     ***** ROTATE FOR PERSPECTIVE TITLE *****                          DRAW0180
  115 Y(3)#W(3)                                                         DRAW0190
      DO 120 I#1,3                                                      DRAW0200
  120 Z(I)#Y(I)-VT(I,4)                                                 DRAW0210
      DO 130 I#1,3                                                      DRAW0220
  130 X(I)#VT(I,1)*Z(1)+VT(I,2)*Z(2)+VT(I,3)*Z(3)+VT(I,4)               DRAW0230
      CALL PLTXY(X,Y)                                                   DRAW0240
C     ***** CHECK BOUNDRY *****                                         DRAW0250
  140 DO 160 J#1,2                                                      DRAW0260
      IF(Y(J)-XLNG(J)+.1)150,150,145                                    DRAW0270
  145 Y(J)#XLNG(J)-.1                                                   DRAW0280
  150 IF(Y(J)-.1)155,160,160                                            DRAW0290
  155 Y(J)#.1                                                           DRAW0300
  160 CONTINUE                                                          DRAW0310
      CALL PLOT(Y(1),Y(2),NPEN)                                         DRAW0320
      RETURN                                                            DRAW0330
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      END                                                               DRAW0340
*LIST8
*LABEL
      SUBROUTINE EIGEN (W,VALU,VECT)                                    EIGE0010
C     ***** EIGENVALUES AND EIGENVECTORS OF 3X3 MATRIX *****            EIGE0020
      DIMENSION W(3,3),VALU(3),VECT(3,3),A(3,3),B(3,3),V(3),U(3)        EIGE0030
      COMMON NG                                                         EIGE0040
C     ***** STATEMENT FUNCTION *****                                    EIGE0050
      PHIF(Z)#((B2-Z)*Z+B1)*Z+B0                                        EIGE0060
C     ***** START OF PROGRAM *****                                      EIGE0070
      ERRND#5.E-8                                                       EIGE0080
      SIGMA#0.                                                          EIGE0090
      DO 115 J#1,3                                                      EIGE0100
      DO 115 I#1,3                                                      EIGE0110
      TEM#W(I,J)                                                        EIGE0120
      A(I,J)#TEM                                                        EIGE0130
  115 SIGMA#SIGMA+TEM*TEM                                               EIGE0140
C     ***** CHECK FOR NULL MATRIX *****                                 EIGE0150
      IF(SIGMA)230,230,120                                              EIGE0160
  120 SIGMA#SQRTF(SIGMA)                                                EIGE0170
C     ***** FORM CHARACTERISTIC EQUATION *****                          EIGE0180
      B2#A(1,1)+A(2,2)+A(3,3)                                           EIGE0190
      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)       EIGE0200
     1+A(2,3)*A(3,2)+A(1,2)*A(2,1)                                      EIGE0210
      B0#A(1,1)*A(2,2)*A(3,3)+A(1,2)*A(2,3)*A(3,1)+A(1,3)*A(3,2)*A(2,1)-EIGE0220
     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)    EIGE0230
C     ***** FIRST ROOT BY BISECTION *****                               EIGE0240
      X#0.                                                              EIGE0250
      Y#SIGMA                                                           EIGE0260
      TEM#PHIF(SIGMA)                                                   EIGE0270
      VNEW#0.0                                                          EIGE0280
      IF(B0)135,250,145                                                 EIGE0290
  135 IF(TEM)140,140,165                                                EIGE0300
  140 Y#-Y                                                              EIGE0310
      GO TO 165                                                         EIGE0320
  145 Y#0.                                                              EIGE0330
      X#SIGMA                                                           EIGE0340
      IF(TEM)165,165,150                                                EIGE0350
  150 X#-X                                                              EIGE0360
C     ***** NOW PHIF(X).LT.0.AND.PHIF(Y).GT.0. *****                    EIGE0370
  165 VNEW#(X+Y)*.5                                                     EIGE0380
      DO 225 I#1,40                                                     EIGE0390
  175 IF(PHIF(VNEW))180,250,185                                         EIGE0400
  180 X#VNEW                                                            EIGE0410
      GO TO 200                                                         EIGE0420
  185 Y#VNEW                                                            EIGE0430
  200 VOLD#VNEW                                                         EIGE0440
      VNEW#(X+Y)*.5                                                     EIGE0450
      TEM#ABSF(VOLD-VNEW)                                               EIGE0460
      IF(TEM-ERRND)250,250,205                                          EIGE0470
  205 IF(VOLD)210,225,210                                               EIGE0480
  210 IF(ABSF(TEM/VOLD)-ERRND)250,250,225                               EIGE0490
  225 CONTINUE                                                          EIGE0500
C     ***** DID NOT CONVERGE, SET ERROR INDICATOR *****                 EIGE0510
  230 NG#6                                                              EIGE0520
      GO TO 400                                                         EIGE0530
C     ***** STORE FIRST ROOT *****                                      EIGE0540
  250 U(3)#VNEW                                                         EIGE0550
C     ***** DEFLATE *****                                               EIGE0560
      C1#B2-VNEW                                                        EIGE0570
      C0#B1+C1*VNEW                                                     EIGE0580
C     ***** SOLVE QUADRATIC *****                                       EIGE0590
      TEM#C1*C1+4.*C0                                                   EIGE0600
      IF(TEM)255,265,260                                                EIGE0610
C     ***** IGNORE IMAGINARY COMPONENT OF COMPLEX ROOT *****            EIGE0620
  255 TEM#0.                                                            EIGE0630
      GO TO 265                                                         EIGE0640
  260 TEM#SQRTF(TEM)                                                    EIGE0650
  265 U(1)#.5*(C1-TEM)                                                  EIGE0660
      U(2)#.5*(C1+TEM)                                                  EIGE0670
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C     ***** SORT ROOTS *****                                            EIGE0680
      DO 275 J#1,2                                                      EIGE0690
      IF(U(J)-U(3))275,275,270                                          EIGE0700
  270 TEM#U(J)                                                          EIGE0710
      U(J)#U(3)                                                         EIGE0720
      U(3)#TEM                                                          EIGE0730
  275 CONTINUE                                                          EIGE0740
      LLL#-2                                                            EIGE0750
      DO 375 III#1,2                                                    EIGE0760
C     ***** CHECK FOR MULTIPLE ROOTS *****                              EIGE0770
      TEM#ERRND*100.                                                    EIGE0780
      NG#0                                                              EIGE0790
      L#1                                                               EIGE0800
      DO 305 I#1,2                                                      EIGE0810
      IF(U(I+1)-U(I)-TEM)300,300,290                                    EIGE0820
  290 IF(U(I))295,305,295                                               EIGE0830
  295 IF(ABSF((U(I+1)-U(I))/U(I))-TEM)300,300,305                       EIGE0840
  300 L#L-1                                                             EIGE0850
      NG#NG-2*I                                                         EIGE0860
  305 CONTINUE                                                          EIGE0870
      IF(LLL-L)308,400,400                                              EIGE0880
  308 LLL#L                                                             EIGE0890
C     ***** EIGENVECTOR ROUTINE *****                                   EIGE0900
      DO 375 II#1,3                                                     EIGE0910
      TI#U(II)                                                          EIGE0920
      IF(L)315,310,322                                                  EIGE0930
C     ***** TWO VECTORS NULL FOR DOUBLE ROOT *****                      EIGE0940
  310 IF(NG+5-II)315,322,315                                            EIGE0950
C     ***** ALL VECTORS NULL FOR TRIPLE ROOT *****                      EIGE0960
  315 DO 320 J#1,3                                                      EIGE0970
  320 VECT(J,II)#0.0                                                    EIGE0980
      GO TO 375                                                         EIGE0990
  322 DO 325 J#1,3                                                      EIGE1000
  325 A(J,J)#W(J,J)-TI                                                  EIGE1010
      SMAX#0.0                                                          EIGE1020
      DO 355 I#1,3                                                      EIGE1030
      II#I                                                              EIGE1040
      IF(I-2)335,335,340                                                EIGE1050
  335 II#I+1                                                            EIGE1060
  340 B(I,1)#A(I,2)*A(II,3)-A(I,3)*A(II,2)                              EIGE1070
      B(I,2)#A(I,3)*A(II,1)-A(I,1)*A(II,3)                              EIGE1080
      B(I,3)#A(I,1)*A(II,2)-A(I,2)*A(II,1)                              EIGE1090
      TEM#B(I,1)**2+B(I,2)**2+B(I,3)**2                                 EIGE1100
      IF(TEM-SMAX)355,355,350                                           EIGE1110
  350 SMAX#TEM                                                          EIGE1120
      IMAX#I                                                            EIGE1130
  355 CONTINUE                                                          EIGE1140
      IF(SMAX)353,353,360                                               EIGE1150
  353 NG#7                                                              EIGE1160
      GO TO 375                                                         EIGE1170
  360 SMAX#SQRTF(SMAX)                                                  EIGE1180
      DO 365 J#1,3                                                      EIGE1190
  365 V(J)#B(IMAX,J)/SMAX                                               EIGE1200
C     ***** REFINE EIGENVECTOR *****                                    EIGE1210
      CALL AXEQB(A,V,V,1)                                               EIGE1220
      TEM#MAXIF(ABSF(V(1)),ABSF(V(2)),ABSF(V(3)))                       EIGE1230
      DO 370 J#1,3                                                      EIGE1240
  370 V(J)#V(J)/TEM                                                     EIGE1250
      CALL UNIT(V,VECT(1,II),1)                                         EIGE1260
C     ***** REFINE EIGENVALUE *****                                     EIGE1270
      TI#VMV(VECT(1,II),W,VECT(1,II))                                   EIGE1280
      U(II)#TI                                                          EIGE1290
  375 VALU(II)#TI                                                       EIGE1300
  400 RETURN                                                            EIGE1310
      END                                                               EIGE1320
*LIST8
*LABEL
      SUBROUTINE ERPNT(TI,N)                                            ERPN0010
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    ERPN0020
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)ERPN0030
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      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) ERPN0040
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) ERPN0050
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   ERPN0060
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   ERPN0070
      DIMENSION XLNG(3),XO(3),XT(3)                                     ERPN0080
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   ERPN0090
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD ERPN0100
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIERPN0110
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   ERPN0120
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                ERPN0130
      WRITE OUTPUT TAPE NOUT,115,NG,TI,N                                ERPN0140
  115 FORMAT(1H 10X,10HFAULT NG #I3,F10.0,I6/1H )                       ERPN0150
      NG#0                                                              ERPN0160
      RETURN                                                            ERPN0170
      END                                                               ERPN0180
*LIST8
*LABEL
      SUBROUTINE F200                                                   F2000010
      DIMENSION PLA(2000)                                               F2000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F2000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F2000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F2000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F2000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F2000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F2000080
      DIMENSION XLNG(3),XO(3),XT(3)                                     F2000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F2000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F2000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF2000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F2000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F2000140
C     ***** CALCOMP CONTROL *****                                       F2000150
      IF(NJ2-1)216,210,212                                              F2000160
  210 CALL PLOTS(PLA(2000),1998,LTNO)                                   F2000170
C     ***** FOR CDC 1604 A USE  210 CALL PLOTS(PLA,2000,LTNO)   *****   F2000175
C     ***** FOR IBM 7090 USE  210 CALL PLOTS(PLA(2000),1998,LTNO)  *****F2000176
      GO TO 216                                                         F2000180
  212 CALL PLOT(AIN(1),AIN(2),-3)                                       F2000190
  216 RETURN                                                            F2000200
      END                                                               F2000210
*LIST8
*LABEL
      SUBROUTINE F400                                                   F4000010
C     ***** ATOM LIST FUNCTIONS *****                                   F4000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F4000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F4000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F4000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F4000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F4000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F4000080
      DIMENSION XLNG(3),XO(3),XT(3)                                     F4000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F4000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F4000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF4000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F4000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F4000140
      NG#0                                                              F4000150
      IF(LATM)402,402,400                                               F4000160
  400 DO 401 I#1,LATM                                                   F4000170
  401 CALL ATOM(ATOMS(1,I),ATOMS(2,I))                                  F4000180
  402 IF(XMODF(NJ2,10)-1)499,404,403                                    F4000190
  403 CALL SEARCH                                                       F4000200
      GO TO 499                                                         F4000210
C     ***** STORES (401) OR REMOVES (411) RUNS OF ATOMS *****           F4000220
C     ***** RUN HIERARCHY # ATOM NO./SYM/ A/B/C TRANS. *****            F4000230
  404 II#1                                                              F4000240
C     ***** FIND RUNS IN AIN ARRAY *****                                F4000250
  405 TI#AIN(II)                                                        F4000260
      IF(TI)410,410,420                                                 F4000270
  410 II#II+1                                                           F4000280
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      IF(140-II)499,405,405                                             F4000290
  420 JJ#II                                                             F4000300
C     ***** SET INITIAL RUN VALUES *****                                F4000310
      MI#TI/100000.                                                     F4000320
      M2#MODF(TI,100.)                                                  F4000330
      M5#MODF(TI/100.,1000.)                                            F4000340
      IF(M5)422,422,423                                                 F4000350
  422 M5#555                                                            F4000360
  423 M3#M5/100                                                         F4000370
      M4#XMODF(M5/10,10)                                                F4000380
      M5#XMODF(M5,10)                                                   F4000390
  425 JJ#JJ+1                                                           F4000400
      IF(140-JJ)435,430,430                                             F4000410
  430 T2#-AIN(JJ)                                                       F4000420
      IF(T2)435,425,440                                                 F4000430
  435 II#JJ-1                                                           F4000440
C     ***** SET TERMINAL VALUES FOR DEGENERATE RUN *****                F4000450
      NI#MI                                                             F4000460
      N2#M2                                                             F4000470
      N3#M3                                                             F4000480
      N4#M4                                                             F4000490
      N5#M5                                                             F4000500
      GO TO 450                                                         F4000510
  440 II#JJ                                                             F4000520
C     ***** SET TERMINAL RUN VALUES *****                               F4000530
      NI#T2/100000.                                                     F4000540
      N2#MODF(T2,100.)                                                  F4000550
      N5#MODF(T2/100.,1000.)                                            F4000560
      IF(N5)445,445,446                                                 F4000570
  445 N5#555                                                            F4000580
  446 N3#N5/100                                                         F4000590
      N4#XMODF(N5/10,10)                                                F4000600
      N5#XMODF(N5,10)                                                   F4000610
C     ***** LOOP THROUGH ALL RUNS *****                                 F4000620
  450 DO 490 L5#M5,N5                                                   F4000630
      DO 490 L4#M4,N4                                                   F4000640
      DO 490 L3#M3,N3                                                   F4000650
      DO 490 L2#M2,N2                                                   F4000660
      DO 490 LI#MI,NI                                                   F4000670
      VI(1)#FLOATF(LI)*100000.+FLOATF(L3*10000+L4*1000+L5*100+L2)       F4000680
      CALL ATOM(VI(1),VI(2))                                            F4000690
      IF(NG)455,458,455                                                 F4000700
  455 CALL ERPNT(VI(1),401)                                             F4000710
      GO TO 490                                                         F4000720
  458 CALL STORE                                                        F4000730
  490 CONTINUE                                                          F4000740
      GO TO 410                                                         F4000750
  499 RETURN                                                            F4000760
      END                                                               F4000770
*LIST8
*LABEL
      SUBROUTINE F500                                                   F5000010
      DIMENSION RM(3,3),V(3,4)                                          F5000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F5000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F5000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F5000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F5000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F5000070
      DIMENSION VT(3,4),VI(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F5000080
      DIMENSION XLNG(3),XO(3),XT(3)                                     F5000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F5000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F5000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF5000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2   F5000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F5000140
      NG#0                                                              F5000150
      IF(NJ2-1)599,501,510                                              F5000160
  501 TI#AIN(1)                                                         F5000170
      CALL ATOM(TI,ORGN)                                                F5000180
      IF(NG)502,504,502                                                 F5000190
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  502 CALL ERPNT(TI,501)                                                F5000200
      CALL EXIT                                                         F5000210
  504 DO 506 K#1,4                                                      F5000220
      TI#AIN(K+1)                                                       F5000230
      CALL ATCM(TI,V(1,K))                                              F5000240
      IF(NG)502,506,502                                                 F5000250
  506 CONTINUE                                                          F5000260
      DO 507 J#1,3                                                      F5000270
      V1(J)#V(J,2)-V(J,1)                                               F5000280
  507 V2(J)#V(J,4)-V(J,3)                                               F5000290
      IND#-1                                                            F5000300
      IF(AIN(7))509,509,508                                             F5000310
  508 IND#-2                                                            F5000320
  509 CALL AXES(V1,V2,REFV,IND)                                         F5000330
      GO TO 562                                                         F5000340
  510 DO 552 L#1,139,2                                                  F5000350
      I#AIN(L)                                                          F5000360
      IF(I)532,552,512                                                  F5000370
  512 X#AIN(L+1)*0.01745329252                                          F5000380
      T1#COSF(X)                                                        F5000390
      T2#SINF(X)                                                        F5000400
      I3#XMODF(I+2,3)+1                                                 F5000410
      I1#XMODF(I3,3)+1                                                  F5000420
      I2#XMODF(I1,3)+1                                                  F5000430
      RM(I1,I1)#T1                                                      F5000440
      RM(I1,I2)#T2                                                      F5000450
      RM(I1,I3)#0.0                                                     F5000460
      RM(I2,I1)#-T2                                                     F5000470
      RM(I2,I2)#T1                                                      F5000480
      RM(I2,I3)#0.0                                                     F5000490
      RM(I3,I1)#0.0                                                     F5000500
      RM(I3,I2)#0.0                                                     F5000510
      RM(I3,I3)#1.0                                                     F5000520
      CALL MM(REFV,RM,V)                                                F5000530
      IF(NJ2-3)518,525,599                                              F5000540
  518 DO 522 J#1,9                                                      F5000550
  522 REFV(J,1)#V(J,1)                                                  F5000560
      GO TO 552                                                         F5000570
  525 DO 528 J#1,9                                                      F5000580
  528 WRKV(J,1)#V(J,1)                                                  F5000590
      GO TO 552                                                         F5000600
  532 IF(NJ2-3)535,552,599                                              F5000610
  535 I#XMODF(-I,3)                                                     F5000620
      DO 542 J#1,I                                                      F5000630
      DO 542 K#1,3                                                      F5000640
      T1#REFV(K,3)                                                      F5000650
      REFV(K,3)#REFV(K,2)                                               F5000660
      REFV(K,2)#REFV(K,1)                                               F5000670
  542 REFV(K,1)#T1                                                      F5000680
  552 CONTINUE                                                          F5000690
      IF(NJ2-3)562,582,599                                              F5000700
  562 CALL MM(AA,REFV,AAREV)                                            F5000710
      DO 572 J#1,9                                                      F5000720
      WRKV(J,1)#REFV(J,1)                                               F5000730
  572 AAWRK(J,1)#AAREV(J,1)                                             F5000740
      GO TO 599                                                         F5000750
  582 CALL MM(AA,WRKV,AAWRK)                                            F5000760
  599 RETURN                                                            F5000770
      END                                                               F5000780
*LIST8
*LABEL
      SUBROUTINE F600                                                   F6000010
C     ***** SCALING AND CENTERING FUNCTIONS *****                       F6000020
      DIMENSION MAX(3),SCAL(4),X(3),XMAX(3),XMIN(3),Z(2)                F6000030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F6000040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F6000050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F6000060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F6000070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F6000080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F6000090
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      DIMENSION XLNG(3),XO(3),XT(3)                                     F6000100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F6000110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F6000120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF6000130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,VI,V2   F6000140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F6000150
C     ***** DEL # 1. FOR INCRUMENTING FUNCTIONS *****                   F6000160
C     ***** DEL # 0. FOR REGULAR FUNCTIONS *****                        F6000170
      DEL#FLOATF(XMODF(NJ2/10,2))                                       F6000180
      NJ2#XMODF(NJ2,10)                                                 F6000190
C     ***** EXPLICIT ORIGIN AND SCALE *****                             F6000200
      IF(AIN(1))602,604,602                                             F6000210
  602 XO(1)#AIN(1)+XO(1)*DEL                                            F6000220
  604 IF(AIN(2))606,608,606                                             F6000230
  606 XO(2)#AIN(2)+XO(2)*DEL                                            F6000240
  608 IF(AIN(3))612,612,609                                             F6000250
  609 IF(DEL)611,611,610                                                F6000260
  610 SCAL1#SCAL1*AIN(3)                                                F6000270
      GO TO 612                                                         F6000280
  611 SCAL1#AIN(3)                                                      F6000290
  612 IF(AIN(4))616,616,614                                             F6000300
C     ***** SET ELLIPSOID SCALE FACTOR *****                            F6000310
  614 SCAL2#AIN(4)                                                      F6000320
C     ***** AUTOMATIC ORIGIN AND/OR SCALE *****                         F6000330
  616 IF(NJ2-2)790,622,620                                              F6000340
  620 XO(1)#XLNG(1)*.5                                                  F6000350
      XO(2)#XLNG(2)*.5                                                  F6000360
  622 IF(NJ2-3)625,640,625                                              F6000370
  625 SCAL1#1.                                                          F6000380
  630 IF(LATM-1)635,635,640                                             F6000390
  635 NG#12                                                             F6000400
      CALL ERPNT(0.,602)                                                F6000410
      CALL EXIT                                                         F6000420
  640 DO 650 J#1,3                                                      F6000430
      XMAX(J)#-1.E5                                                     F6000440
  650 XMIN(J)#1.E5                                                      F6000450
C     ***** FIT BOX AROUND SET OF ATOMS *****                           F6000460
      DO 670 I#1,LATM                                                   F6000470
      CALL XYZ(ATOMS(1,I),ATOMS(2,I),3)                                 F6000480
      IF(NG)652,653,652                                                 F6000490
  652 CALL ERPNT(ATOMS(1,I),600)                                        F6000500
      GO TO 670                                                         F6000510
  653 DO 668 J#1,3                                                      F6000520
      TI#ATOMS(J+1,I)                                                   F6000530
      IF(XMAX(J)-TI)655,660,660                                         F6000540
  655 XMAX(J)#TI                                                        F6000550
      MAX(J)#I                                                          F6000560
  660 IF(TI-XMIN(J))665,668,668                                         F6000570
  665 XMIN(J)#TI                                                        F6000580
  668 CONTINUE                                                          F6000590
  670 CONTINUE                                                          F6000600
C     ***** KM#TOP ATOM *****                                           F6000610
      KM#MAX(3)                                                         F6000620
      SMULT#1.                                                          F6000630
      DO 780 M#1,5                                                      F6000640
      IF(M-2)740,675,678                                                F6000650
C     ***** CHECK VIEW DISTANCE *****                                   F6000660
  675 IF(VIEW)785,785,680                                               F6000670
  678 IF(NJ2-3)680,785,680                                              F6000680
  680 TI#ATOMS(4,KM)*SMULT                                              F6000690
      IF(VIEW*.5-TI)685,690,690                                         F6000700
C     ***** INCREASE VIEW DISTANCE *****                                F6000710
  685 VIEW#2.*TI                                                        F6000720
C     ***** FIND PERSPECTIVE PROJECTION LIMITS *****                    F6000730
  690 DO 700 J#1,2                                                      F6000740
      XMAX(J)#-1.E5                                                     F6000750
  700 XMIN(J)#1.E5                                                      F6000760
      DO 725 I#1,LATM                                                   F6000770
      DO 705 J#1,3                                                      F6000780
  705 X(J)#ATOMS(J+1.I)*SMULT                                           F6000790
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      T2#VIEW/(VIEW-X(3))                                               F6000800
      DO 725 J#1,2                                                      F6000810
      T1#X(J)*T2                                                        F6000820
      IF(XMAX(J)-T1)710,715,715                                         F6000830
  710 XMAX(J)#T1                                                        F6000840
  715 IF(T1-XMIN(J))720,725,725                                         F6000850
  720 XMIN(J)#T1                                                        F6000860
  725 CONTINUE                                                          F6000870
C     ***** REFINE PARAMETERS *****                                     F6000880
  740 IF(NJ2 -3)745,742,755                                             F6000890
  742 SMUL2#1.                                                          F6000900
      GO TO 765                                                         F6000910
C     ***** AUTOMATIC SCALE ONLY *****                                  F6000920
  745 DO 750 J#1,2                                                      F6000930
      T2#XO(J)                                                          F6000940
      SCAL(J)#(BRDR-T2)/XMIN(J)                                         F6000950
  750 SCAL(J+2)#(XLNG(J)-BRDR-T2)/XMAX(J)                               F6000960
      SMUL2#MIN1F(SCAL(1),SCAL(2),SCAL(3),SCAL(4))                      F6000970
      GO TO 780                                                         F6000980
C     ***** AUTOMATIC SCALE AND POSITION *****                          F6000990
  755 DO 760 J#1,2                                                      F6001000
  760 SCAL(J)#(XLNG(J)-BRDR*2.)/(XMAX(J)-XMIN(J))                       F6001010
      SMUL2#MIN1F(SCAL(1),SCAL(2))                                      F6001020
C     ***** AUTOMATIC POSITION *****                                    F6001030
  765 DO 770 J#1,2                                                      F6001040
  770 XO(J)#.5*(XLNG(J)-SMUL2*(XMAX(J)+XMIN(J)))                        F6001050
  780 SMULT#SMULT*SMUL2                                                 F6001060
      VIEW#VIEW*SMUL2                                                   F6001070
  785 SCAL1#SCAL1*SMULT                                                 F6001080
  790 SCL#SCAL1*SCAL2                                                   F6001090
      RETURN                                                            F6001100
      END                                                               F6001110
*LIST8
*LABEL
      SUBROUTINE F700                                                   F7000010
C     ***** SUBROUTINE TO DRAW ELLIPSOIDS *****                         F7000020
      DIMENSION EYE(3),VIEWV(3),X(3),Z(3)                               F7000030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F7000040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F7000050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F7000060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F7000070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F7000080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F7000090
      DIMENSION XLNG(3),XO(3),XT(3)                                     F7000100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F7000110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F7000120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1F7000130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F7000140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F7000150
C     ***** SET ELLIPSOID GRAPHIC DETAILS *****                         F7000160
      ITILT#0                                                           F7000170
      NG#0                                                              F7000180
      NFIRST#1                                                          F7000190
      NPLANE#AIN(1)                                                     F7000200
      IF(NPLANE-1)720,715,720                                           F7000210
  715 NFIRST#4                                                          F7000220
      NPLANE#4                                                          F7000230
  720 NSOLID#AIN(2)                                                     F7000240
      NDCT#64/2**(XABSF(NSOLID))                                        F7000250
      LINES#AIN(3)                                                      F7000260
      NDASH#AIN(4)                                                      F7000270
      CHSYM#AIN(5)                                                      F7000280
      DH#AIN(6)-CHSYM*17./7.                                            F7000290
      DV#AIN(7)-CHSYM*.5                                                F7000300
C     ***** ESTABLISH REFERENCE POINT OF VIEW *****                     F7000310
      T1#1.E6                                                           F7000320
      IF(VIEW)740,740,735                                               F7000330
  735 T1#VIEW/SCAL1                                                     F7000340
  740 DO 745 J#1,3                                                      F7000350
  745 EYE(J)#REFV(J,3)*T1+ORGN(J)                                       F7000360
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      LNS#-1                                                            F7000370
C     ***** LCOP THROUGH ATOM LIST *****                                F7000380
      DO 1105 ITOM#1,LATM                                               F7000390
      TI#ATOMS(I,ITOM)                                                  F7000400
      CALL XYZ(TI,X,2)                                                  F7000410
      IF(NG)758,746,758                                                 F7000420
  746 CALL PLTXY(X,Z)                                                   F7000430
      K#TI/100000.                                                      F7000440
      L#TI-FLOATF(K)*100000.                                            F7000450
      IF(NJ2-10)747,754,754                                             F7000460
  747 LNS#XMODF(LNS+1,18)                                               F7000470
      IF(LNS)749,748,749                                                F7000480
  748 WRITE OUTPUT TAPE NOUT,751,(TITLE(I),I#1,12)                      F7000490
      WRITE OUTPUT TAPE NOUT,752                                        F7000500
  749 WRITE OUTPUT TAPE NOUT,750,CHEM(K),K,L,Z(1),Z(2),(X(I),I#1,3),(XT(F7000510
     11),I#1,3)                                                         F7000520
  750 FORMAT(1H 10X,A6,3H  (I3,1H,I5,4H)   2F8.2,3X,3F8.3,11X,3F8.4)    F7000530
  751 FORMAT(1H11 0X,12A6)                                              F7000540
  752 FORMAT(1H31 0X,18HSYMBOL   ATOM CODE7X,16HPLOTTER X,Y(IN.) 3X,21HCAF7000550
     1RTESIAN X,Y,Z (IN.)15X,20HCRYSTAL SYSTEM X,Y,Z/1H 19X,45H(DIRECTIOF7000560
     2N COSINES(I,J),I#1,3),RMSD(J)),J#1,312X,42HFOR PRINCIPAL AXES BASEF7000570
     3D CN WORKING SYSTEM/1H )                                          F7000580
  754 IF(EDGE-BRDR*.75)755,760,760                                      F7000590
  755 NG#10                                                             F7000600
  758 CALL ERPNT(TI,700)                                                F7000610
      GO TO 1105                                                        F7000620
  760 IF(CHSYM)775,775,765                                              F7000630
C     ***** PLOT CHEMICAL SYMBOLS *****                                 F7000640
  765 T4#1.                                                             F7000650
      IF(VIEW)767,767,766                                               F7000660
  766 T4#VIEW/(VIEW-X(3))                                               F7000670
  767 T3#CHSYM*T4                                                       F7000680
      T4#DISP*T4*.5                                                     F7000690
      V1(1)#X(1)+DH*SYMB(1,1)+DV*SYMB(1,2)                              F7000700
      V1(2)#X(2)+DH*SYMB(2,1)+DV*SYMB(2,2)                              F7000710
      V1(3)#X(3)                                                        F7000720
      CALL PLTXY(V1,V3)                                                 F7000730
      IF(EDGE-CHSYM)775,768,768                                         F7000740
  768 V2(3)#0.                                                          F7000750
      DO 770 I#1,3,2                                                    F7000760
      V2(1)#V3(1)+FLOATF(I-2)*T4                                        F7000770
      DO 770 J#1,3,2                                                    F7000780
      V2(2)#V3(2)+FLOATF(J-2)*T4                                        F7000790
      CALL SIMBOL(V2(1),V2(2),T3,CHEM(K),THETA,6)                       F7000800
      IF(T4)775,775,770                                                 F7000810
  770 CONTINUE                                                          F7000820
  775 IF(NPLANE)1105,1105,780                                           F7000830
C     ***** ELLIPSOID PRINC VECTORS TOWARD VIEWER *****                 F7000840
  780 CALL PAXES(TI,2)                                                  F7000850
      IF(NG)758,783,758                                                 F7000860
  783 CALL DIFV(EYE,XT,VIEWV)                                           F7000870
      CALL UNIT(VIEWV,VIEWV,-1)                                         F7000880
      CALL VM(VIEWV,AA,V2)                                              F7000890
      DO 795 I#1,3                                                      F7000900
      IF(VV(V2,PAT(1,I)))785,795,795                                    F7000910
  785 DO 790 J#1,3                                                      F7000920
      PAC(J,I)#-PAC(J,I)                                                F7000930
  790 PAT(J,I)#-PAT(J,I)                                                F7000940
  795 CONTINUE                                                          F7000950
      DO 800 J#1,3                                                      F7000960
      PAC(J,4)#PAC(J,1)                                                 F7000970
  800 PAC(J,5)#PAC(J,2)                                                 F7000980
      IF(NJ2-10)802,803,803                                             F7000990
  801 FORMAT(1H 13X,3(3X,3F8.4,F8.5)/1H )                               F7001000
  802 WRITE OUTPUT TAPE NOUT,801,(((PAC(J,K),J#1,3),RMS(K)),K#1,3)      F7001010
C     ***** V4 # VECTOR NORMAL TO POLAR PLANE *****                     F7001020
  803 CALL VM(VIEWV,AAWRK,V6)                                           F7001030
      CALL UNIT(V6,V6,1)                                                F7001040
      CALL MV(Q,V6,V4)                                                  F7001050
      CALL UNIT(V4,V4,1)                                                F7001060
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C     ***** SET PLOTTING RESOLUTION FOR ELLIPSOID *****                F7001070
      T3#RMS(3)*SCL                                                    F7001080
      NRESOL#1                                                         F7001090
      NBIS#5                                                           F7001100
      DO 805 J#1,3                                                     F7001110
      IF(T3-RES(J))804,810,810                                         F7001120
  804 NBIS#NBIS-1                                                      F7001130
  805 NRESOL#NRESOL*2                                                  F7001140
  810 NRES1#NRESOL+1                                                   F7001150
C     ***** LOOP THROUGH PRINC AND POLAR PLANES *****                  F7001160
      DO 1100 II#NFIRST,NPLANE                                         F7001170
      II0#XMODF(II+2,3)+1                                              F7001180
      III#XMODF(II,3)+1                                                F7001190
      II2#XMODF(II+1,3)+1                                              F7001200
C     ***** GENERATE CONJUGATE DIAMETERS *****                         F7001210
      IF(.99938-ABSF(VV(V4,PAC(1,II2))))820,820,830                    F7001220
  820 T1#RMS(II0)*SCL                                                  F7001230
      T2#RMS(III)*SCL                                                  F7001240
      DO 825 J#1,3                                                     F7001250
      DA(J,1)#PAC(J,II0)*T1                                            F7001260
  825 DA(J,2)#PAC(J,III)*T2                                            F7001270
      GO TO 850                                                        F7001280
  830 CALL NORM(PAC(1,II0),PAC(1,III),V1,1)                            F7001290
      CALL NORM(V1,V4,V2,1)                                            F7001300
      CALL UNIT(V2,V2,1)                                               F7001310
      CALL MV(Q,V2,V3)                                                 F7001320
      IF(II-4)835,840,840                                              F7001330
  835 CALL NORM(V3,V1,V5,1)                                            F7001340
      GO TO 843                                                        F7001350
  840 CALL NORM(V3,V4,V5,1)                                            F7001360
  843 CALL UNIT(V5,V5,1)                                               F7001370
      T1#SCL/SQRTF(VMV(V2,Q,V2))                                       F7001380
      T2#SCL/SQRTF(VMV(V5,Q,V5))                                       F7001390
      DO 845 J#1,3                                                     F7001400
      DA(J,1)#V2(J)*T1                                                 F7001410
  845 DA(J,2)#V5(J)*T2                                                 F7001420
C     ***** GENERATE ELLIPSE *****                                     F7001430
  850 CALL RADIAL(NBIS)                                                F7001440
      IF(II-4)900,855,855                                              F7001450
C     ***** PLOT BOUNDARY ELLIPSE *****                                F7001460
  855 CALL PROJ(D,DP,X,X0,VIEW,1,129,NRESOL)                           F7001470
      CALL DRAW(DP,0.,0.,3)                                            F7001480
      DO 860 J#NRES1,129,NRESOL                                        F7001490
  860 CALL DRAW(DP(1,J),0.,0.,2)                                       F7001500
      IF(DISP)1100,1100,865                                            F7001510
C     ***** BOUNDARY ANNULUS AS A LINEAR FUNCTION OF HEIGHT *****      F7001520
  865 CALL DIFV(XT,ORGN,V1)                                            F7001530
      T5#VV(V1,AAREV(1,3))*SCAL1                                       F7001540
      NCYCLE#.5+(AIN(8)+T5*AIN(9))/DISP                                F7001550
      IF(NCYCLE)1100,1100,870                                          F7001560
  870 T3#(2.*DISP)/(T1+T2)                                             F7001570
C     ***** INCREASE ANNULAR THICKNESS *****                           F7001580
      DO 875 I#1,NCYCLE                                                F7001590
      T4#T3*FLOATF(I)                                                  F7001600
      DO 875 J#1,129,NRESOL                                            F7001610
  875 CALL DRAW(DP(1,J),D(1,J)*T4,D(2,J)*T4,2)                         F7001620
      GO TO 1100                                                       F7001630
  900 CALL PROJ(D,DP,X,X0,VIEW,1,65,NRESOL)                            F7001640
C     ***** PLOT HALF AN ELLIPSE *****                                 F7001650
      CALL DRAW(DP,0.,0.,3)                                            F7001660
      DO 905 J#NRES1,65,NRESOL                                         F7001670
  905 CALL DRAW(DP(1,J),0.,0.,2)                                       F7001680
      IF(DISP)930,930,910                                              F7001690
C     ***** ACCENTUATE FRONT HALF *****                                F7001700
  910 DO 925 I#1,3,2                                                   F7001710
      T2#FLOATF(I-2)*DISP                                              F7001720
      DO 915 J#1,65,NRESOL                                             F7001730
      K#66-J                                                           F7001740
  915 CALL DRAW(DP(1,K),DISP,T2,2)                                     F7001750
      DO 925 K#1,65,NRESOL                                             F7001760
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  925 CALL DRAW(DP(1,K),-DISP,-T2,2)                                    F7001770
  930 IF(NSOLID)940,967,935                                             F7001780
  935 L#NDOT                                                            F7001790
      IF(NDOT-NRESOL)938,945,940                                        F7001800
  938 CALL RADIAL(NSOLID-1)                                             F7001810
      GO TO 945                                                         F7001820
  940 L#NRESOL                                                          F7001830
  945 CALL PROJ(D(1,65),DP(1,65),X,XO,VIEW,1,65,L)                      F7001840
      IF(NSOLID)960,967,950                                             F7001850
C     ***** DOTTED LINE ON REVERSE SIDE *****                           F7001860
  950 DO 958 J#65,129,NDOT                                              F7001870
      CALL DRAW(DP(1,J),DISP,DISP,3)                                    F7001880
      DO 955 I#1,3,2                                                    F7001890
      T1#FLOATF(I-2)*DISP                                               F7001900
      DO 955 K#1,3,2                                                    F7001910
      T2#FLOATF(K-2)*DISP                                               F7001920
      CALL DRAW(DP(1,J),T1,T2,2)                                        F7001930
      IF(DISP)958,958,955                                               F7001940
  955 CONTINUE                                                          F7001950
  958 CONTINUE                                                          F7001960
      GO TO 967                                                         F7001970
C     ***** SINGLE LINE ON REVERSE SIDE *****                           F7001980
  960 DO 965 J#65,129,NRESOL                                            F7001990
  965 CALL DRAW(DP(1,J),0.,0.,2)                                        F7002000
C     ***** DETAIL INTERIOR FEATURES *****                              F7002010
  967 T2#NDASH*2                                                        F7002020
      DO 975 J#1,3                                                      F7002030
      T1#PAC(J,110)*RMS(110)*SCL                                        F7002040
      DA(J,1)#T1                                                        F7002050
      DA(J,2)#PAC(J,111)*RMS(111)*SCL                                   F7002060
      DA(J,3)#0.                                                        F7002070
      IF(NDASH)975,975,970                                              F7002080
  970 V1(J)#-T1                                                         F7002090
      V2(J)#T1/T2                                                       F7002100
  975 CONTINUE                                                          F7002110
      IF(NDASH)987,987,980                                              F7002120
C     ***** DASHED LINE FOR REVERSE AXIS *****                          F7002130
  980 DO 985 J#1,NDASH                                                  F7002140
      DO 985 K#1,2                                                      F7002150
      L#4-K                                                             F7002160
      CALL PROJ(V1,DP,X,XO,VIEW,1,1,1)                                  F7002170
      CALL DRAW(DP,0.,0.,L)                                             F7002180
      DO 985 I#1,3                                                      F7002190
  985 V1(I)#V1(I)+V2(I)                                                 F7002200
C     ***** SOLID LINE FOR FORWARD AXIS *****                           F7002210
  987 IF(LINES)1100,1100,988                                            F7002220
  988 CALL PROJ(DA,DP,X,XO,VIEW,1,3,1)                                  F7002230
      T1#DISP*.5                                                        F7002240
      DO 990 I#1,3,2                                                    F7002250
      T2#FLOATF(2-I)*T1                                                 F7002260
      CALL DRAW(DP,T1,T2,3)                                             F7002270
      CALL DRAW(DP(1,3),T1,T2,2)                                        F7002280
      IF(DISP)1000,1000,989                                             F7002290
  989 CALL DRAW(DP(1,3),-T1,T2,2)                                       F7002300
  990 CALL DRAW(DP,-T1,T2,2)                                            F7002310
C     ***** SHADE QUADRANT BETWEEN TWO PRINCIPAL AXES *****             F7002320
 1000 L#LINES-1                                                         F7002330
      IF(L)1100,1100,1005                                               F7002340
 1005 T2#LINES                                                          F7002350
      DO 1025 I#1,L                                                     F7002360
      T1#FLOATF(I)/T2                                                   F7002370
      T3#SQRTF(1.-T1*T1)                                                F7002380
      IF(XMODF(I,2))1010,1015,1010                                      F7002390
 1010 M#I*2                                                             F7002400
      N#M-1                                                             F7002410
      GO TO 1020                                                        F7002420
 1015 N#I*2                                                             F7002430
      M#N-1                                                             F7002440
 1020 DO 1025 J#1,3                                                     F7002450
      T4#DA(J,1)*T1                                                     F7002460
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      D(J,M)#T4                                                         F7002470
 1025 D(J,N)#DA(J,2)*T3+T4                                              F7002480
      L#L*2                                                             F7002490
      CALL PRCJ(D,DP,X,XO,VIEW,1,L,1)                                   F7002500
      DO 1030 I#2,L,2                                                   F7002510
      CALL DRAW(DP(1,I-1),0.,0.,3)                                      F7002520
 1030 CALL DRAW(DP(1,I),0.,0.,2)                                        F7002530
 1100 CONTINUE                                                          F7002540
 1105 CONTINUE                                                          F7002550
      RETURN                                                            F7002560
      END                                                               F7002570
*LIST8
*LABEL
      SUBROUTINE F800                                                   F8000010
C     ***** SUBROUTINE FINDS ATOM PAIRS FOR BONDS *****                 F8000020
      DIMENSION IA(3),WI(3)                                             F8000030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    F8000040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F8000050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F8000060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F8000070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F8000080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F8000090
      DIMENSION XLNG(3),XO(3),XT(3)                                     F8000100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F8000110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F8000120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF8000130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F8000140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                F8000150
      LNS#-4                                                            F8000160
      IF(XMODF(NJ2,10)-2)805,840,840                                    F8000170
C     ***** EXPLICIT DESCRIPTION *****                                  F8000180
  805 II#0                                                              F8000190
      IF(NCD)845,845,815                                                F8000200
  815 II#II+1                                                           F8000210
      IF(140-II)899,899,820                                             F8000220
  820 T1#AIN(II)                                                        F8000230
      IF(T1)815,815,825                                                 F8000240
  825 II#II+1                                                           F8000250
      T2#AIN(II)                                                        F8000260
      IF(T2)815,815,830                                                 F8000270
  830 IF(NJ2-10)832,838,838                                             F8000280
  832 LNS#XMODF(LNS+4,56)                                               F8000290
      IF(LNS)838,834,838                                                F8000300
  834 WRITE OUTPUT TAPE NOUT,835,(TITLE(I),I#1,12)                      F8000310
  835 FORMAT(1H110X,12A6)                                               F8000320
      WRITE OUTPUT TAPE NOUT,837                                        F8000330
  837 FORMAT(1H010X,18HSYMBOL   ATOM CODE6X,16HPLOTTER X,Y(IN.) 6X,21HCAF8000340
     1RTESIAN X,Y,Z (IN.)17X,20HCRYSTAL SYSTEM X,Y,Z/1H )               F8000350
  838 CALL BOND(T1,T2,1)                                                F8000360
      GO TO 815                                                         F8000370
C     ***** IMPLICIT DESCRIPTION *****                                  F8000380
  840 IF(LATM-2)845,850,850                                             F8000390
  845 NG#11                                                             F8000400
      CALL ERPNT(0.,NJ*100+NJ2)                                         F8000410
      GO TO 899                                                         F8000420
  850 SCAL3#SCAL1                                                       F8000430
      SCAL1#1.                                                          F8000440
      DO 855 I#1,LATM                                                   F8000450
  855 CALL XYZ(ATOMS(1,I),ATOMS(2,I),2)                                 F8000460
      SCAL1#SCAL3                                                       F8000470
      IF(NCD)845,845,860                                                F8000480
  860 WRITE OUTPUT TAPE NOUT,861                                        F8000490
  861 FORMAT(1H010X,20HBOND SELECTION CODES//11X,94H(SEQUENCE(A))(SEQUENF8000500
     1CE(B)) (BCND) (DISTANCES)( BOND )(PERSP.--LABELS)(NORMAL--LABELS)(F8000510
     2DIGITS) /11X,93H(  MIN  MAX )(  MIN  MAX ) (TYPE) (MIN   MAX)(RADIF8000520
     3US)(HEIGHT  OFFSET)(HEIGHT  OFFSET)(NUMBER))                      F8000530
      DMAX#0.                                                           F8000540
      DO 870 I#1,NCD                                                    F8000550
      IF(DMAX-CD(2,I))865,870,870                                       F8000560
  865 DMAX#CD(2,I)                                                      F8000570
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  870 WRITE OUTPUT TAPE NOUT,871,(KD(J,I),J#1,5),(CD(J,I),J#1,8)          F8000580
  871 FORMAT(1H 10X16,I5,I8,I5,I8,2F6.2,5F8.3,F7.0)                       F8000590
      DMAX#DMAX*DMAX                                                      F8000600
C     ***** LOOP THROUGH ATOMS ARRAY *****                                F8000610
      DO 895 M#1,LATM                                                     F8000620
      T1#ATOMS(1,M)                                                       F8000630
      IA(1)#T1/100000.                                                    F8000640
      IA(3)#IA(1)                                                         F8000650
      W1(1)#ATOMS(2,M)                                                    F8000660
      W1(2)#ATOMS(3,M)                                                    F8000670
      W1(3)#ATOMS(4,M)                                                    F8000680
      L#M+1                                                               F8000690
      DO 895 N#L,LATM                                                     F8000700
      DIST#(ATOMS(2,N)-W1(1))**2                                          F8000710
      IF(DMAX-DIST)895,873,873                                            F8000720
  873 DIST#DIST+(ATOMS(3,N)-W1(2))**2                                     F8000730
      IF(DMAX-DIST)895,874,874                                            F8000740
  874 DIST#DIST+(ATOMS(4,N)-W1(3))**2                                     F8000750
      IF(DMAX-DIST)895,875,875                                            F8000760
  875 DIST#SQRTF(DIST)                                                    F8000770
      T2#ATOMS(1,N)                                                       F8000780
      IA(2)#T2/100000.                                                    F8000790
C     ***** SELECT BONDS ACCORDING TO CODES *****                         F8000800
      DO 890 J#1,NCD                                                      F8000810
      JB#J                                                                F8000820
      IF(DIST-CD(1,J))    890,880,880                                     F8000830
  880 IF(CD(2,J)-DIST)    890,881,881                                     F8000840
  881 DO 885 K#1,2                                                        F8000850
      IF(IA(K)-KD(1,J))   885,882,882                                     F8000860
  882 IF(KD(2,J)-IA(K))   885,883,883                                     F8000870
  883 IF(IA(K+1)-KD(3,J))885,884,884                                      F8000880
  884 IF(KD(4,J)-IA(K+1))885,891,891                                      F8000890
  885 CONTINUE                                                            F8000900
  890 CONTINUE                                                            F8000910
      GO TO 895                                                           F8000920
  891 IF(NJ2-10)892,894,894                                               F8000930
  892 LNS#XMODF(LNS+4,56)                                                 F8000940
      IF(LNS)893,893,894                                                  F8000950
  893 WRITE OUTPUT TAPE NOUT,835,(TITLE(I),I#1,12)                        F8000960
      WRITE OUTPUT TAPE NOUT,837                                          F8000970
  894 CALL BOND(T1,T2,JB)                                                 F8000980
  895 CONTINUE                                                            F8000990
  899 RETURN                                                              F8001000
      END                                                                 F8001010
*LIST8
*LABEL
      SUBROUTINE F900                                                     F9000010
      DIMENSION X(3),XW(3,5),Y(3),Z(3)                                    F9000020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)      F9000030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)F9000040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) F9000050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) F9000060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   F9000070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   F9000080
      DIMENSION XLNG(3),XO(3),XT(3)                                       F9000090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   F9000100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD F9000110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIF9000120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   F9000130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                  F9000140
C     ***** LABELING FUNCTION SUBROUTINE *****                            F9000150
      ITILT#0                                                             F9000160
      NJ3#XMODF(NJ2,10)                                                   F9000170
      TH#THETA                                                            F9000180
      SINTH#SYMB(2,1)                                                     F9000190
      COSTH#SYMB(1,1)                                                     F9000200
      ILAST#1                                                             F9000210
      IF(AIN(2)-11100.)910,910,905                                        F9000220
  905 ILAST#2                                                             F9000230
  910 DO 925 II#1,ILAST                                                   F9000240
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C     ***** OBTAIN WORKING CARTESIAN COORDINATES *****                F9000250
      CALL XYZ(AIN(II),XW(1,II),2)                                     F9000260
      IF(NG)915,925,915                                                F9000270
  912 NG#15                                                            F9000280
  915 CALL ERPNT(AIN(II),NJ*100+NJ2)                                   F9000290
      GO TO 1199                                                       F9000300
  925 CALL XYZ(AIN(II),XW(1,II+3),3)                                   F9000310
      II#1                                                             F9000320
C     ***** FIND MEAN REFERENCE POINT *****                            F9000330
      DO 930 J#1,3                                                     F9000340
      T2#XW(J,ILAST)                                                   F9000350
      T1#XW(J,1)                                                       F9000360
      XW(J,3)#T2-T1                                                    F9000370
  930 X(J)#(T2+T1)*.5                                                  F9000380
C     ***** PERSPECTIVE SCALING FACTOR *****                           F9000390
      SCAL#1.                                                          F9000400
      IF(VIEW)940,940,935                                              F9000410
  935 SCAL#VIEW/(VIEW-X(3))                                            F9000420
  940 HGT#SCAL*AIN(5)                                                  F9000430
      IF(NJ2-3)960,950,945                                             F9000440
  945 IF(NJ2-6)950,950,960                                             F9000450
C     ***** PROJECTED VECTOR BASELINE *****                            F9000460
  950 CALL PLTXY(XW(1,4),V1)                                           F9000470
      CALL PLTXY(XW(1,5),V2)                                           F9000480
      T1#V2(1)-V1(1)                                                   F9000490
      T2#V2(2)-V1(2)                                                   F9000500
      T3#SQRTF(T1*T1+T2*T2)                                            F9000510
      IF(T3)912,912,955                                                F9000520
  955 COSTH#T1/T3                                                      F9000530
      SINTH#T2/T3                                                      F9000540
      TH#ARCCOS(COSTH)                                                 F9000550
      IF(SINTH)958,960,960                                             F9000560
  958 TH#-TH                                                           F9000570
  960 IF(NJ2-13)965,985,985                                            F9000580
C     ***** FIND CENTER OF PROJECTED LABEL *****                       F9000590
  965 Y(1)#SCAL*(X(1)+AIN(6)*COSTH-AIN(7)*SINTH)+XO(1)                 F9000600
      Y(2)#SCAL*(X(2)+AIN(6)*SINTH+AIN(7)*COSTH)+XO(2)                 F9000610
      Y(3)#0.                                                          F9000620
C     ***** CHECK FOR LEGEND RESET *****                               F9000630
      DO 980 J#1,2                                                     F9000640
      T1#AIN(J+2)                                                      F9000650
      IF(T1)975,980,970                                                F9000660
  970 Y(J)#T1                                                          F9000670
      GO TO 980                                                        F9000680
  975 Y(J)#XLNG(J)+T1                                                  F9000690
  980 CONTINUE                                                         F9000700
C     ***** SET PARAMETERS FOR INDIVIDUAL FUNCTIONS *****              F9000710
  985 GO TO(990,995,995,1000,1000,1000,915,1105,1105,915,915,915,1005,10F9000720
     105,1005,1005,915),NJ2                                            F9000730
  990 T6#17.                                                           F9000740
      L#AIN(1)/100000.                                                 F9000750
      ILAST#1                                                          F9000760
      DXW#0.                                                           F9000770
      DYW#0.                                                           F9000780
      GO TO 1030                                                       F9000790
  995 T6#215.                                                          F9000800
      ILAST#12                                                         F9000810
      T1#HGT*36./7.                                                    F9000820
      DXW#COSTH*T1                                                     F9000830
      DYW#SINTH*T1                                                     F9000840
      GO TO 1030                                                       F9000850
 1000 T6#22+3*(6-NJ3)                                                  F9000860
      DIST#SQRTF(VV(XW(1,3),XW(1,3)))/SCAL1                            F9000870
      GO TO 1030                                                       F9000880
C     ***** TRUE PERSPECTIVE LABELS *****                              F9000890
 1005 CALL UNIT(XW(1,3),VT(1,1),1)                                     F9000900
      IF(ABSF(VT(3,1))-.9994)1010,912,912                              F9000910
C     ***** FORM PERSPECTIVE ROTATION MATRIX *****                     F9000920
 1010 CALL NORM(AID(1,3),VT(1,1),VT(1,2),1)                            F9000930
      CALL UNIT(VT(1,2),VT(1,2),1)                                     F9000940
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      CALL NORM(VT(1,1),VT(1,2),VT(1,3),1)                              F9000950
      DO 1015 J#1,3                                                     F9000960
 1015 VT(J,4)#X(J)                                                      F9000970
      ITILT#1                                                           F9000980
      HGT#AIN(5)                                                        F9000990
      TH#0.                                                             F9001000
      Y(3)#X(3)                                                         F9001010
      Y(2)#X(2)+AIN(7)-HGT*.5                                           F9001020
      IF(NJ2-13)1030,1025,1020                                          F9001030
C     ***** PERSPECTIVE BCND LABELS *****                               F9001040
 1020 Y(1)#X(1)+AIN(6)-HGT*FLOATF(22+3*(6-NJ3))/7.                      F9001050
      DIST#SQRTF(VV(XW(1,3),XW(1,3)))/SCALI                             F9001060
      GO TO 1050                                                        F9001070
C     ***** PERSPECTIVE TITLES *****                                    F9001080
 1025 Y(1)#X(1)+AIN(6)-HGT*215./7.                                      F9001090
      ILAST#12                                                          F9001100
      DXW#HGT*36./7.                                                    F9001110
      DYW#0.                                                            F9001120
      GO TO 1050                                                        F9001130
 1030 DH#HGT*T6/7.                                                      F9001140
      DV#HGT*.5                                                         F9001150
      Y(1)#Y(1)-DH*COSTH+DV*SINTH                                       F9001160
      Y(2)#Y(2)-DH*SINTH-DV*COSTH                                       F9001170
      Y(3)#0.                                                           F9001180
C     ***** PLOT VARIOUS LABELS *****                                   F9001190
 1050 GO TO(1060,1060,1060,1090,1095,1100,915,1105,1105),NJ3            F9001200
 1060 DO 1085 I#1,ILAST                                                 F9001210
      DO 1075 J#1,3,2                                                   F9001220
      Z(1)#Y(1)+FLOATF(J-2)*DISP*.5                                     F9001230
      DO 1075 K#1,3,2                                                   F9001240
      Z(2)#Y(2)+FLOATF(K-2)*DISP*.5                                     F9001250
      IF(NJ3-2)1065,1068,1068                                           F9001260
C     ***** PLOT CHEMICAL SYMBOL *****                                  F9001270
 1065 CALL SIMBOL(Z(1),Z(2),HGT,CHEM(L),TH,6)                           F9001280
      GO TO 1070                                                        F9001290
C     ***** PLOT TITLES *****                                           F9001300
 1068 CALL SIMBOL(Z(1),Z(2),HGT,TITLE2(I),TH,6)                         F9001310
 1070 IF(DISP)1080,1080,1075                                            F9001320
 1075 CONTINUE                                                          F9001330
 1080 Y(1)#Y(1)+DXW                                                     F9001340
 1085 Y(2)#Y(2)+DYW                                                     F9001350
      GO TO 1199                                                        F9001360
C     ***** PLOT BCND DISTANCE LABELS *****                             F9001370
 1090 CALL NOMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.1)                         F9001380
      GO TO 1199                                                        F9001390
 1095 CALL NOMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.2)                         F9001400
      GO TO 1199                                                        F9001410
 1100 CALL NOMBER(Y(1),Y(2),HGT,DIST,TH,4HF6.3)                         F9001420
      GO TO 1199                                                        F9001430
C     ***** PLOT CENTERED SYMBOLS *****                                 F9001440
 1105 CALL SIMBOL(Y(1),Y(2),HGT,XFIXF(AIN(8)),TH,7-NJ3)                 F9001450
 1199 ITILT#0                                                           F9001460
      RETURN                                                            F9001470
      END                                                               F9001480
*LIST8
*LABEL
      SUBROUTINE F1000                                                  F10C0010
      RETURN                                                            F10C0020
      END                                                               F10C0030
*LIST8
*LABEL
      SUBROUTINE MM(X,Y,Z)                                              MM  0010
C     MULTIPLY TWO MATRICES                                             MM  0020
C     Z(3,3)#X(3,3)*Y(3,3)                                              MM  0030
      DIMENSIONX(3,3),Y(3,3),Z(3,3)                                     MM  0040
      DO117I#1,3                                                        MM  0050
      DO117K#1,3                                                        MM  0060
      Z(I,K)#0.0                                                        MM  0070
      DO117J#1,3                                                        MM  0080
  117 Z(I,K)#Z(I,K)+X(I,J)*Y(J,K)                                       MM  0090
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      RETURN                                                            MM  0100
      END                                                               MM  0110
*LIST8
*LABEL
      SUBROUTINE MV(X,Y,Z)                                              MV  0010
C     MATRIX * VECTOR                                                   MV  0020
C     Z(3)#X(3,3)*Y(3)                                                  MV  0030
      DIMENSICNX(3,3),Y(3),Z(3)                                         MV  0040
      DO113I#1,3                                                        MV  0050
      Z(I)#0.0                                                          MV  0060
      DO113J#1,3                                                        MV  0070
  113 Z(I)#Z(I)+X(I,J)*Y(J)                                             MV  0080
      RETURN                                                            MV  0090
      END                                                               MV  0100
*LIST8
*LABEL
      SUBROUTINE NORM(X,Y,Z,ITYPE)                                      NORM0010
C     ***** VECTOR PRODUCT  Z#X*Y *****                                 NORM0020
C     ***** ITYPE .GT.0 FOR CARTESIAN,.LE.0 FOR TRICLINIC *****         NORM0030
      DIMENSICN X(3),Y(3),Z(3,3),ZI(3,3)                                NORM0040
      DIMENSICN A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    NORM0050
      DIMENSICN ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)NORM0060
      DIMENSICN DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) NORM0070
      DIMENSICN P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) NORM0080
      DIMENSICN RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   NORM0090
      DIMENSICN VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   NORM0100
      DIMENSICN XLNG(3),XO(3),XT(3)                                     NORM0110
      COMMCN NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   NORM0120
      COMMCN DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD NORM0130
      COMMCN NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALINORM0140
      COMMCN SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   NORM0150
      COMMCN V3,V4,V5,V6,WRKV,XLNG,XO,XT                                NORM0160
      DO 125 I#1,3                                                      NORM0170
      I1#XMODF(I+3,3)+1                                                 NORM0180
      I2#XMODF(I+1,3)+1                                                 NORM0190
      T1#X(I1)*Y(I2)-X(I2)*Y(I1)                                        NORM0200
      IF(ITYPE)115,115,105                                              NORM0210
  105 Z(I)#T1                                                           NORM0220
      GO TO 125                                                         NORM0230
  115 ZI(I)#T1                                                          NORM0240
  125 CCNTINUE                                                          NORM0250
      IF(ITYPE)135,135,300                                              NORM0260
  135 CALL MV(BB,ZI,Z)                                                  NORM0270
  300 RETURN                                                            NORM0280
      END                                                               NORM0290
*LIST8
*LABEL
      SUBROUTINE PAXES(ACODE,ITYPE)                                     PAXE0010
C     ***** ITYPE .LT.0 FOR COVARIANCE MATRIX IN Q *****                PAXE0020
C     ***** ITYPE .GT.0 FOR ELLIPSOID QUADRATIC FORM IN Q *****         PAXE0030
C     ***** XABSF(ITYPE)#1 BASED ON TRICLINIC COORDINATE SYSTEM *****   PAXE0040
C     ***** #2 OR 3 FOR WORKING OR REFERENCE CARTESIAN SYSTEMS *****    PAXE0050
C     ***** CHECK ATOM CODE *****                                       PAXE0060
      DIMENSICN W(3,3),X(3)                                             PAXE0070
      DIMENSICN A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PAXE0080
      DIMENSICN ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PAXE0090
      DIMENSICN DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PAXE0100
      DIMENSICN P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PAXE0110
      DIMENSICN RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PAXE0120
      DIMENSICN VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PAXE0130
      DIMENSICN XLNG(3),XO(3),XT(3)                                     PAXE0140
      COMMCN NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PAXE0150
      COMMCN DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PAXE0160
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPAXE0170
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PAXE0180
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PAXE0190
      IT#XABSF(ITYPE)-1                                                 PAXE0200
      KS#MODF(ACODE,100.)                                               PAXE0210
      IF(NSYM-KS)105,115,115                                            PAXE0220
  105 NG#4                                                              PAXE0230
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      GO TO 300                                                         PAXE0240
  115 II#ACODE/100000.                                                  PAXE0250
      IF(NATOM-II)125,130,130                                           PAXE0260
  125 NG#5                                                              PAXE0270
      GO TO 300                                                         PAXE0280
  130 IF(II)125,125,135                                                 PAXE0290
C     ***** CRYSTALLOGRAPHIC SYMMETRY ROTATION *****                    PAXE0300
  135 CALL TMM(PA(1,1,II),FS(1,1,KS),PAT)                               PAXE0310
      IF(IT-1)165,145,155                                               PAXE0320
C     ***** TRANSFORM TO CARTESIAN SYSTEMS *****                        PAXE0330
  145 CALL TMM(PAT,AAWRK,PAC)                                           PAXE0340
      GO TO 175                                                         PAXE0350
  155 CALL TMM(PAT,AAREV,PAC)                                           PAXE0360
      GO TO 175                                                         PAXE0370
  165 IF(ITYPE)170,175,170                                              PAXE0380
C     ***** (PAT)**(-1) * (AA)**(-1) *****                              PAXE0390
  170 CALL AXEQB(PAT,W,BB,3)                                            PAXE0400
C     ***** FORM DIAGONAL MATRIX OR ITS INVERSE *****                   PAXE0410
  175 DO 205 J#1,3                                                      PAXE0420
      TI#EV(J,II)                                                       PAXE0430
      IF(ITYPE)195,205,185                                              PAXE0440
  185 X(J)#1./(TI*TI)                                                   PAXE0450
      GO TO 205                                                         PAXE0460
  195 X(J)#TI*TI                                                        PAXE0470
  205 RMS(J)#TI                                                         PAXE0480
C     ***** FORM QUADRATIC FORM *****                                   PAXE0490
      DO 245 I#1,3                                                      PAXE0500
      DO 245 J#I,3                                                      PAXE0510
      TI#0.0                                                            PAXE0520
      IF(IT)300,210,220                                                 PAXE0530
  210 DO 215 K#1,3                                                      PAXE0540
C     ***** BASED ON TRICLINIC SYSTEM *****                             PAXE0550
  215 TI#TI+PAT(I,K)*W(K,J)*X(K)                                        PAXE0560
      GO TO 235                                                         PAXE0570
C     ***** BASED ON CARTESIAN SYSTEM *****                             PAXE0580
  220 DO 225 K#1,3                                                      PAXE0590
  225 TI#TI+PAC(I,K)*PAC(J,K)*X(K)                                      PAXE0600
  235 Q(J,I)#TI                                                         PAXE0610
  245 Q(I,J)#TI                                                         PAXE0620
  300 RETURN                                                            PAXE0630
      END                                                               PAXE0640
*LIST8
*LABEL
      SUBROUTINE PLTXY(X,Y)                                             PLTX0010
C     ***** PLOT COORD. AND CLOSEST EDGE AFTER PROJECTION *****         PLTX0020
      DIMENSION X(3),Y(2)                                               PLTX0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PLTX0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PLTX0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PLTX0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PLTX0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PLTX0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PLTX0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     PLTX0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PLTX0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PLTX0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPLTX0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PLTX0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PLTX0150
      T4#1.                                                             PLTX0160
      TI#1.                                                             PLTX0170
      IF(VIEW)125,125,110                                               PLTX0180
  110 T4#VIEW-X(3)                                                      PLTX0190
      IF(T4)115,115,120                                                 PLTX0200
  115 Y(1)#-99.                                                         PLTX0210
      Y(2)#-99.                                                         PLTX0220
      GO TO 130                                                         PLTX0230
  120 TI#VIEW/T4                                                        PLTX0240
  125 Y(1)#X(1)*TI+XO(1)                                                PLTX0250
      Y(2)#X(2)*TI+XO(2)                                                PLTX0260
      TI#XLNG(1)-ABSF(Y(1)*2.-XLNG(1))                                  PLTX0270
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      T2#XLNG(2)-ABSF(Y(2)*2.-XLNG(2))                                  PLTX0280
      EDGE#MINIF(T1,T2)*.5                                              PLTX0290
      IF(T4-VIEW*.5)130,300,300                                         PLTX0300
  130 EDGE#-99.                                                         PLTX0310
  300 RETURN                                                            PLTX0320
      END                                                               PLTX0330
*LIST8
*LABEL
      SUBROUTINE PRELIM                                                 PREL0010
C     ***** DATA INPUT ROUTINE *****                                    PREL0020
      DIMENSION B(9)                                                    PREL0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PREL0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PREL0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PREL0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PREL0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PREL0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PREL0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     PREL0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PREL0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATN,LTNO,NATOM,NCD PREL0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPREL0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PREL0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PREL0150
C     ***** CELL DIMENSIONS *****                                       PREL0160
  106 FORMAT(6F9.6)                                                     PREL0170
      READ INPUT TAPE IN,106,(A(I),I#1,6)                               PREL0180
      T1#ABSF(A(4))-1.                                                  PREL0190
      DO 125 J#1,3                                                      PREL0200
      IF(T1)115,110,110                                                 PREL0210
C     ***** CELL ANGLES IN DEGREES *****                                PREL0220
  110 A(J+6)#A(J+3)                                                     PREL0230
      A(J+3)#COSF(A(J+6)*.01745329252)                                  PREL0240
      GO TO 120                                                         PREL0250
C     ***** COSINES OF CELL ANGLES *****                                PREL0260
  115 A(J+6)#ARCCOS(A(J+3))                                             PREL0270
C     ***** STORE IDEMFACTOR MATRIX *****                               PREL0280
  120 AID(J,J)#1.                                                       PREL0290
      AID(J+1,1)#0.                                                     PREL0300
      AID(J+5,1)#0.                                                     PREL0310
C     ***** STORE METRIC TENSOR *****                                   PREL0320
  125 AA(J,J)#A(J)**2                                                   PREL0330
      AA(1,2)#A(1)*A(2)*A(6)                                            PREL0340
      AA(1,3)#A(1)*A(3)*A(5)                                            PREL0350
      AA(2,3)#A(2)*A(3)*A(4)                                            PREL0360
      AA(2,1)#AA(1,2)                                                   PREL0370
      AA(3,1)#AA(1,3)                                                   PREL0380
      AA(3,2)#AA(2,3)                                                   PREL0390
C     ***** INVERT METRIC TENSOR *****                                  PREL0400
      CALL AXEQB(AA,BB,AID,3)                                           PREL0410
C     ***** CALCULATE RECIPROCAL CELL PARAMETERS *****                  PREL0420
      DO 128 J#1,3                                                      PREL0430
  128 B(J)#SQRTF(BB(J,J))                                               PREL0440
      B(6)#BB(1,2)/(B(1)*B(2))                                          PREL0450
      B(5)#BB(1,3)/(B(1)*B(3))                                          PREL0460
      B(4)#BB(2,3)/(B(2)*B(3))                                          PREL0470
      DO 130 J#1,3                                                      PREL0480
  130 B(J+6)#ARCCOS(B(J+3))                                             PREL0490
C     ***** WAS INPUT FOR REAL OR RECIPROCAL CELL *****                 PREL0500
      IF(A(1)-1.)135,150,150                                            PREL0510
  135 DO 140 J#1,9                                                      PREL0520
      T1#AA(J,1)                                                        PREL0530
      AA(J,1)#BB(J,1)                                                   PREL0540
      BB(J,1)#T1                                                        PREL0550
      T1#A(J)                                                           PREL0560
      A(J)#B(J)                                                         PREL0570
  140 B(J)#T1                                                           PREL0580
C     ***** WRITE OUT CELL PARAMETERS *****                             PREL0590
  143 FORMAT(1H0 10X,22HDIRECT CELL PARAMETERS/1H 15X,1HA14X,1HB14X,1HC14PREL0600
     1X,5HALPHA10X,4HBETA11X,5HGAMMA)                                   PREL0610
  145 FORMAT(1H 10X,F9.6,2F15.6,3F15.3/1H 48X,6HCOSINEF12.8,2F15.8)     PREL0620
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  147 FORMAT(1H010X,26HRECIPROCAL CELL PARAMETERS/1H 15X,2HA*13X,2HB*13XPREL0630
     1,2HC*13X,6HALPHA*9X,5HBETA*10X,6HGAMMA*)                          PREL0640
  150 WRITE OUTPUT TAPE NOUT,143                                        PREL0650
      WRITE OUTPUT TAPE NOUT,145,(A(I),I#1,3),(A(I),I#7,9),(A(I),I#4,6) PREL0660
      WRITE OUTPUT TAPE NOUT,147                                        PREL0670
      WRITE OUTPUT TAPE NOUT,145,(B(I),I#1,3),(B(I),I#7,9),(B(I),I#4,6) PREL0680
C     ***** STORE STANDARD VECTORS *****                                PREL0690
      CALL AXES(AID,AID(1,2),REFV,0)                                    PREL0700
      CALL MM(AA,REFV,AAREV)                                            PREL0710
      DO 160 I#1,3                                                      PREL0720
      DO 160 J#1,3                                                      PREL0730
      AAWRK(J,I)#AAREV(J,I)                                             PREL0740
      Q(J,I)#REFV(I,J)                                                  PREL0750
  160 WRKV(J,I)#REFV(J,I)                                               PREL0760
C     ***** READ AND WRITE SYMMETRY TRANSFORMATIONS *****               PREL0770
  171 FORMAT(1H010X,24HSYMMETRY TRANSFORMATIONS/1H 14X,3HNO.12X,13HTRANSPREL0780
     1FORMED X18X,13HTRANSFORMED Y18X,13HTRANSFORMED Z)                 PREL0790
  173 FORMAT(I1,F14.10,3F3.0,2(F15.10,3F3.0))                           PREL0800
  175 FORMAT(1H 13X,I2,3(F13.6,F4.0,2H XF4.0,2H YF4.0,2H Z))            PREL0810
  177 FORMAT(1H110X,12A6)                                               PREL0820
      WRITE OUTPUT TAPE NOUT,171                                        PREL0830
      LINES#14                                                          PREL0840
      DO 190 I#1,48                                                     PREL0850
      LINES#XMODF(LINES+1,56)                                           PREL0860
      READ INPUT TAPE IN,173,IS,(TS(J,I),(FS(K,J,I),K#1,3),J#1,3)       PREL0870
      IF(LINES)185,180,185                                              PREL0880
  180 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12)                      PREL0890
      WRITE OUTPUT TAPE NOUT,171                                        PREL0900
  185 WRITE OUTPUT TAPE NOUT,175,I,(TS(J,I),(FS(K,J,I),K#1,3),J#1,3)    PREL0910
C     ***** NON-CRYSTALLOGRAPHIC HELIX-SYMMETRY INPUT *****             PREL0920
      IF(FS(3,3,I)-5.)188,186,186                                       PREL0930
  186 T1#FS(1,3,I)/FS(3,3,I)                                            PREL0940
      TS(3,I)#TS(3,I)+T1                                                PREL0950
      T1#MODF(T1*FS(2,3,I),1.)*6.28318531                               PREL0960
      T2#COSF(T1)                                                       PREL0970
      T1#SINF(T1)                                                       PREL0980
      DO 187 J#1,9                                                      PREL0990
  187 VT(J,I)#AID(J,I)                                                  PREL1000
      VT(1,1)#T2                                                        PREL1010
      VT(2,2)#T2                                                        PREL1020
      VT(2,1)#-T1                                                       PREL1030
      VT(1,2)#T1                                                        PREL1040
      CALL MM(VT,Q,PAC)                                                 PREL1050
      CALL MM(AAREV,PAC,FS(1,1,I))                                      PREL1060
  188 IF(IS)195,190,195                                                 PREL1070
  190 CONTINUE                                                          PREL1080
      NG#1                                                              PREL1090
      CALL ERPNT(0.,0)                                                  PREL1100
      I#48                                                              PREL1110
  195 NSYM#I                                                            PREL1120
C     ***** POSITIONAL AND THERMAL PARAMETERS *****                     PREL1130
  207 FORMAT(11H0 NO. ATOM 8X,1HX10X,1HY10X,1HZ13X,3HB118X,3HB228X,3HB33PREL1140
     18X,3HB128X,3HB138X,10HB23   TYPE)                                 PREL1150
  209 FORMAT(1H I3,1X,A6,3F11.6,5X,6F11.6,F5.0)                         PREL1160
  210 FORMAT(1H I3,1X,A6,3F11.6,5X,2F11.6,4F11.0,F5.0)                  PREL1170
  211 FORMAT(A6,3X,5F9.6,F9.0)                                          PREL1180
  213 FORMAT(I1,F8.6,5F9.6,F9.0)                                        PREL1190
      LINES#LINES+2                                                     PREL1200
      IF(LINES-56)220,215,215                                           PREL1210
  215 LINES#-1                                                          PREL1220
      GO TO 225                                                         PREL1230
  220 WRITE OUTPUT TAPE NOUT,207                                        PREL1240
  225 DO 245 I#1,200                                                    PREL1250
      LINES#XMODF(LINES+1,56)                                           PREL1260
      READ INPUT TAPE IN,211,CHEM(I),V1(1),V1(2),(P(J,I),J#1,3),T1      PREL1270
      K#1.+T1                                                           PREL1280
      READ INPUT TAPE IN,213,IS,(PA(J,1,I),J#1,7)                       PREL1290
      IF(LINES)230,230,232                                              PREL1300
  230 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12)                      PREL1310
      WRITE OUTPUT TAPE NOUT,207                                        PREL1320
```

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  232 IF(PA(3,1,I)-10000.)235,234,234                                   PREL1330
  234 WRITE OUTPUT TAPE NOUT,210,I,CHEM(I),(P(J,I),J#1,3),(PA(J,1,I),J#1PREL1340
     1,7)                                                               PREL1350
      GO TO 238                                                         PREL1360
  235 WRITE OUTPUT TAPE NOUT,209,I,CHEM(I),(P(J,I),J#1,3),(PA(J,1,I),J#1PREL1370
     1,7)                                                               PREL1380
  238 GO TO (244,239,241,242,244),K                                     PREL1390
C     ***** TYPE 1 POSITICNAL PARAMETERS (ANGSTROMS) *****              PREL1400
  239 DO 240 J#1,3                                                      PREL1410
  240 P(J,I)#P(J,I)/A(J)                                                PREL1420
      GO TO 244                                                         PREL1430
C     ***** TYPE 2 POSITICNAL PARAMETERS, STANDARD CARTESIAN *****      PREL1440
  241 VI(1)#P(1,I)                                                      PREL1450
      VI(2)#P(2,I)                                                      PREL1460
      GO TO 243                                                         PREL1470
C     ***** TYPE 3 POSITICNAL PARAMETERS *****                          PREL1480
C     ***** CYLINDRICAL COORDINATES REFERRED TO STANDARD CARTESIAN *****PREL1490
  242 T2#P(2,I)*.01745329252                                            PREL1500
      VI(1)#VI(1)+P(1,I)*COSF(T2)                                       PREL1510
      VI(2)#VI(2)+P(1,I)*SINF(T2)                                       PREL1520
  243 VI(3)#P(3,I)                                                      PREL1530
      CALL VM(VI,Q,P(1,I))                                              PREL1540
  244 IF(IS)246,245,246                                                 PREL1550
  245 CONTINUE                                                          PREL1560
      NG#2                                                              PREL1570
      CALL ERPNT(0.,0)                                                  PREL1580
      I#200                                                             PREL1590
  246 NATOM#I                                                           PREL1600
C     ***** CONVERT TEMP FACTOR COEF TO STANDARD TYPE ZERO *****        PREL1610
      NGI#0                                                             PREL1620
      DO 450 I#1,NATOM                                                  PREL1630
      TI#PA(1,1,I)                                                      PREL1640
      K#1.+PA(7,1,I)                                                    PREL1650
      IF(TI)250,250,255                                                 PREL1660
  250 TI#.1                                                             PREL1670
      GO TO 405                                                         PREL1680
  255 T6#.0506605918                                                    PREL1690
      GO TO(270,260,265,265,270,260,400,405,999),K                      PREL1700
C     ***** TYPE 1 *****                                                PREL1710
  260 DO 262 J#4,6                                                      PREL1720
  262 PA(J,1,I)#PA(J,1,I)*.5                                            PREL1730
      GO TO 270                                                         PREL1740
C     ***** TYPES 2 AND 3 (BASE 2 SYSTEMS) *****                        PREL1750
  265 T6#.351152464                                                     PREL1760
      IF(K-4)270,260,270                                                PREL1770
C     ***** TYPES 0 THROUGH 5 *****                                     PREL1780
  270 IF(PA(2,1,I))400,400,272                                          PREL1790
  272 DO 300 J#1,3                                                      PREL1800
      DO 300 L#J,3                                                      PREL1810
      T2#T6                                                             PREL1820
      IF(K-5)285,275,275                                                PREL1830
C     ***** TYPES 4 AND 5 *****                                         PREL1840
  275 T2#B(J)*B(L)*T2*.25                                               PREL1850
  285 IF(J-L)290,282,290                                                PREL1860
  282 VT(J,J)#T2*PA(J,1,I)                                              PREL1870
      GO TO 300                                                         PREL1880
  290 M#J+L+1                                                           PREL1890
      VT(J,L)#T2*PA(M,1,I)                                              PREL1900
      VT(L,J)#VT(J,L)                                                   PREL1910
  300 CONTINUE                                                          PREL1920
C     ***** FIND PRINCIPAL AXES *****                                   PREL1930
      CALL MM(VT,AA,DA)                                                 PREL1940
      CALL EIGEN(DA,RMS,PAT)                                            PREL1950
C     ***** ARE EIGENVALUES POSITIVE *****                              PREL1960
      IF(RMS(1))325,325,320                                             PREL1970
  320 IF(NG)350,360,330                                                 PREL1980
  325 NG#3                                                              PREL1990
  330 NGI#1                                                             PREL2000
      CALL ERPNT(FLOATF(I)*100000.+55501.,0)                            PREL2010
C     ***** 3 EQUAL EIGENVALUES, USE REFERENCE VECTORS *****            PREL2020
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  340 T3#SIGNF(SQRTF(ABSF(RMS(1)+RMS(2)+RMS(3))/3.),RMS(1))                PREL2030
      DO 345 J#1,3                                                         PREL2040
      DO 342 K#1,3                                                         PREL2050
  342 PA(J,K,I)#REFV(J,K)                                                  PREL2060
  345 EV(J,I)#T3                                                           PREL2070
      GO TO 450                                                            PREL2080
  350 IF(NG+6)340,340,352                                                  PREL2090
C     ***** TWO EQUAL EIGENVALUES *****                                    PREL2100
  352 N#NG+5                                                               PREL2110
      CALL UNIT(PAT(1,N),V1,-1)                                            PREL2120
      DO 354 K#1,3                                                         PREL2130
      IF(ABSF(VMV(V1,AA,REFV(1,K)))-.58)356,354,354                        PREL2140
  354 CONTINUE                                                             PREL2150
  356 CALL MM(AA,DA,VT)                                                    PREL2160
      CALL AXES(V1,REFV(1,K),DA,-1)                                        PREL2170
      DO 359 K#1,3                                                         PREL2180
      L#XMODF(N+K-2,3)+1                                                   PREL2190
      DO 358 J#1,3                                                         PREL2200
  358 PA(J,L,I)#DA(J,K)                                                    PREL2210
  359 EV(L,I)#SIGNF(SQRTF(ABSF(VMV(DA(1,K),VT,DA(1,K)))),RMS(L))           PREL2220
      GO TO 450                                                            PREL2230
C     ***** MAKE EIGENVECTORS 1 ANGSTROM LONG *****                        PREL2240
  360 DO 365 J#1,3                                                         PREL2250
  365 CALL UNIT(PAT(1,J),PA(1,J,I),-1)                                     PREL2260
  370 NG#0                                                                 PREL2270
C     ***** SQRT EIGENVALUE # RMS DISPLACEMENT *****                       PREL2280
      DO 375 J#1,3                                                         PREL2290
      T2#RMS(J)                                                            PREL2300
  375 EV(J,I)#SIGNF(SQRTF(ABSF(T2)),T2)                                    PREL2310
      GO TO 450                                                            PREL2320
C     ***** TYPE 6 (ISOTROPIC TEMP FACTOR) *****                           PREL2330
  400 T1#SQRTF(T1*.012665148)                                              PREL2340
C     ***** TYPE 7 (DUMMY SPHERE) *****                                    PREL2350
  405 DO 410 J#1,3                                                         PREL2360
  410 EV(J,I)#T1                                                           PREL2370
      IF(PA(3,1,I))430,430,415                                             PREL2380
C     ***** DEFINED VECTORS FOR SPHERE *****                               PREL2390
  415 DO 425 J#1,4                                                         PREL2400
      T2#PA(J+2,1,I)                                                       PREL2410
      CALL ATOM(T2,VT(1,J))                                                PREL2420
      IF(NG)420,425,420                                                    PREL2430
  420 CALL ERPNT(T2,0)                                                     PREL2440
      GO TO 430                                                            PREL2450
  425 CCONTINUE                                                            PREL2460
      CALL DIFV(VT(1,2),VT(1,1),V1)                                        PREL2470
      CALL DIFV(VT(1,4),VT(1,3),V2)                                        PREL2480
      CALL AXES(V1,V2,PA(1,1,I),-1)                                        PREL2490
      GO TO 450                                                            PREL2500
C     ***** REFERENCE VECTORS FOR SPHERE *****                             PREL2510
  430 DO 435 J#1,9                                                         PREL2520
  435 PA(J,1,I)#REFV(J,1)                                                  PREL2530
  450 NG#0                                                                 PREL2540
C     ***** WRITE OUT RMS VALUES *****                                     PREL2550
      LINES#LINES+2                                                        PREL2560
      IF(LINES-56)458,458,455                                              PREL2570
  455 LINES#-1                                                             PREL2580
      GO TO 460                                                            PREL2590
  458 WRITE OUTPUT TAPE NOUT,461                                           PREL2600
  460 DO 465 I#1,NATOM                                                     PREL2610
      LINES#XMODF(LINES+1,56)                                              PREL2620
      IF(LINES)465,462,465                                                 PREL2630
  461 FORMAT(10HONO. ATOM 8X,1HX10X,1HY10X,1HZ13X,7HRMSD 1 4X,7HRMSD 2 4PREL2640
     1X,7HRMSD 3 )                                                         PREL2650
  462 WRITE OUTPUT TAPE NOUT,177,(TITLE(J),J#1,12)                         PREL2660
      WRITE OUTPUT TAPE NOUT,461                                           PREL2670
  463 FORMAT(1H I3,1X,A6,3F11.6)                                           PREL2680
  465 WRITE OUTPUT TAPE NOUT,209,I,CHEM(I),(P(J,I),J#1,3),(EV(J,I),J#1,3PREL2690
     1)                                                                    PREL2700
      IF(NG1)999,999,470                                                   PREL2710
  470 CALL EXIT                                                            PREL2720
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  999 RETURN                                                            PREL2730
      END                                                               PREL2740
*LIST8
*LABEL
      SUBROUTINE PRIME                                                  PRIM0010
C     ****GENERAL INITIALIZATICN OF PRIME PARAMETERS****                PRIM0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    PRIM0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)PRIM0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) PRIM0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) PRIM0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   PRIM0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   PRIM0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     PRIM0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   PRIM0100
      COMMCN DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD PRIM0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIPRIM0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   PRIM0130
      COMMCN V3,V4,V5,V6,WRKV,XLNG,XO,XT                                PRIM0140
      BRDR#0.5                                                          PRIM0150
C     ****CALCULATE CONSTANTS****                                       PRIM0160
      DO 2999 I#1,5                                                     PRIM0170
 2999 CONT(I)#SQRTF(1./(2.*(1.+COSF(3.141592654/2.**I))))               PRIM0180
      DISP#.005                                                         PRIM0190
      FORE#.866                                                         PRIM0200
      IN#10                                                             PRIM0210
      ITILT#0                                                           PRIM0220
      LATM#0                                                            PRIM0230
      LTNO#23                                                           PRIM0240
      NCD#0                                                             PRIM0250
      NG#0                                                              PRIM0260
      NOUT#9                                                            PRIM0270
      NSR#11                                                            PRIM0280
      RES(1)#1.25                                                       PRIM0290
      RES(2)#.5                                                         PRIM0300
      RES(3)#.2                                                         PRIM0310
      SCAL1#1.0                                                         PRIM0320
      SCAL2#1.54                                                        PRIM0330
      SCL#1.54                                                          PRIM0340
      DO 3000 I#1,3                                                     PRIM0350
      SYMB(I,I)#1.                                                      PRIM0360
      SYMB(I+1,I)#0.                                                    PRIM0370
 3000 SYMB(I+5,I)#0.                                                    PRIM0380
      TAPER#.375                                                        PRIM0390
      THETA#0.0                                                         PRIM0400
      VIEW#0.0                                                          PRIM0410
      XLNG(1)#30.0                                                      PRIM0420
      XLNG(2)#11.0                                                      PRIM0430
      XO(1)#15.0                                                        PRIM0440
      XO(2)#5.5                                                         PRIM0450
      RETURN                                                            PRIM0460
      END                                                               PRIM0470
*LIST8
*LABEL
      SUBROUTINE PROJ(D,DP,X,XO,VIEW,I1,I2,I3)                          PROJ0010
C     ***** 3D CARTESIAN TO 2D PLOTTER COORDINATES *****                PROJ0020
      DIMENSION D(3,129),DP(2,129),X(3),XO(3)                           PROJ0030
      T3#VIEW-X(3)                                                      PROJ0040
      DO 145 I#I1,I2,I3                                                 PROJ0050
      T1#D(1,I)+X(1)                                                    PROJ0060
      T2#D(2,I)+X(2)                                                    PROJ0070
      IF(VIEW)135,135,120                                               PROJ0080
  120 T4#VIEW/(T3-D(3,I))                                               PROJ0090
      T1#T1*T4                                                          PROJ0100
      T2#T2*T4                                                          PROJ0110
  135 DP(1,I)#T1+XO(1)                                                  PROJ0120
  145 DP(2,I)#T2+XO(2)                                                  PROJ0130
      RETURN                                                            PROJ0140
      END                                                               PROJ0150
*LIST8
*LABEL
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      SUBROUTINE RADIAL(ND)                                             RADI0010
C     ***** GENERATE ELLIPSE FROM TWO CONJUGATE VECTORS *****           RADI0020
C     ***** ORTHONORMAL VECTORS PRODUCE 8-128 SPOKED CIRCLE *****       RADI0030
C     ***** ND DENOTES NUMBER OF SUBDIVISIONS (1 TO 5) *****            RADI0040
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    RADI0050
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)RADI0060
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) RADI0070
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) RADI0080
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   RADI0090
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   RADI0100
      DIMENSION XLNG(3),XO(3),XT(3)                                     RADI0110
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   RADI0120
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD RADI0130
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIRADI0140
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   RADI0150
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                RADI0160
      DO 115 J#1,3                                                      RADI0170
      T1#DA(J,1)                                                        RADI0180
      D(J,1)#T1                                                         RADI0190
      D(J,129)#T1                                                       RADI0200
      D(J,65)#-T1                                                       RADI0210
      T1#DA(J,2)                                                        RADI0220
      D(J,33)#T1                                                        RADI0230
  115 D(J,97)#-T1                                                       RADI0240
      DO 135 K#1,ND                                                     RADI0250
      T1#CONT(K)                                                        RADI0260
      KDEL#2**(6-K)                                                     RADI0270
      KDEL1#KDEL+1                                                      RADI0280
      KDEL2#KDEL/2                                                      RADI0290
      DO 135 L#KDEL1,65,KDEL                                            RADI0300
      J#L-KDEL                                                          RADI0310
      M#L-KDEL2                                                         RADI0320
      DO 135 N#1,3                                                      RADI0330
      T2#(D(N,L)+D(N,J))*T1                                             RADI0340
      D(N,M)#T2                                                         RADI0350
  135 D(N,M+64)#-T2                                                     RADI0360
      RETURN                                                            RADI0370
      END                                                               RADI0380
*LIST8
*LABEL
      SUBROUTINE SEARCH                                                 SEAR0010
      DIMENSION NW(6),DX(3),S(2,200),U(3),V(3),W(2,4),WW(2,3),X(4),Y(3) SEAR0020
      DIMENSION Z(3)                                                    SEAR0030
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    SEAR0040
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)SEAR0050
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) SEAR0060
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) SEAR0070
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   SEAR0080
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   SEAR0090
      DIMENSION XLNG(3),XO(3),XT(3)                                     SEAR0100
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   SEAR0110
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD SEAR0120
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALISEAR0130
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   SEAR0140
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                SEAR0150
      EQUIVALENCE(NW(1),LL),(NW(2),LU),(NW(3),ML)                       SEAR0160
      EQUIVALENCE(NW(4),MU),(NW(5),NL),(NW(6),NU)                       SEAR0170
C     ***** OBTAIN PROBLEM PARAMETERS *****                             SEAR0180
      WRITE OUTPUT TAPE NOUT,20                                         SEAR0190
   20 FORMAT(1H0 9X,82H       FROM ATOMS     TO ATOMS        WITH RADIUS ORSEAR0200
     1, IF A BOX, WITH SEMIDIMENSIONS  /11X,46HCODE (MIN   MAX)    (MIN   MSEAR0210
     2AX)                    7X,1HA8X,1HB8X,1HC)                        SEAR0220
      IF(AIN(1)-10000.)100,100,101                                      SEAR0230
  100 ITCM1#AIN(1)                                                      SEAR0240
      SYITOM#55501.                                                     SEAR0250
      GO TO 103                                                         SEAR0260
  101 ITCM1#AIN(1)/100000.                                              SEAR0270
      SYITOM#MODF(AIN(1),100000.)                                       SEAR0280
  102 IF(AIN(2)-10000.)103,103,104                                      SEAR0290
  103 ITCM2#AIN(2)                                                      SEAR0300
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      GO TO 105                                                         SEAR0310
  104 ITOM2#AIN(2)/100000.                                              SEAR0320
  105 ITAR1#AIN(3)                                                      SEAR0330
      IF(ITAR1)108,108,110                                              SEAR0340
  108 ITAR1#1                                                           SEAR0350
  110 ITAR2#AIN(4)                                                      SEAR0360
      DMAX#AIN(5)                                                       SEAR0370
      IF(DMAX)115,115,120                                               SEAR0380
  115 DMAX#4.                                                           SEAR0390
      AIN(5)#DMAX                                                       SEAR0400
  120 DMX#DMAX*DMAX                                                     SEAR0410
      TEM#.01                                                           SEAR0420
      KFUN#NJ*100+XMODF(NJ2,10)                                         SEAR0430
      K#NJ*100+NJ2                                                      SEAR0440
      I0#SYITOM                                                         SEAR0450
  121 FORMAT(1H010X,2I3,2I5,I7,I5,18X,3F9.3/1H )                        SEAR0460
      WRITE OUTPUT TAPE NOUT,121,K,ITOM1,I0,ITOM2,ITAR1,ITAR2,(AIN(J),J#SEAR0470
     15,7)                                                              SEAR0480
  124 FORMAT(1H 15X,2I5,I8,I5,2F9.3)                                    SEAR0490
      IF(NCD)130,130,125                                                SEAR0500
  125 WRITE OUTPUT TAPE NOUT,124,(((KD(J,I),J#1,4),(CD(J,I),J#1,2)),I#1,SEAR0510
     1NCD)                                                              SEAR0520
  130 DO 135 J#1,4                                                      SEAR0530
      W(1,J)#99.                                                        SEAR0540
  135 W(2,J)#-99.                                                       SEAR0550
      DO 155 I#ITAR1,ITAR2                                              SEAR0560
      T1#FLOATF(I)*100000.                                              SEAR0570
      CALL ATOM(T1,X)                                                   SEAR0580
      IF(NG)140,145,140                                                 SEAR0590
  140 CALL ERPNT(T1,KFUN)                                               SEAR0600
      GO TO 600                                                         SEAR0610
  145 X(4)#X(1)-X(2)                                                    SEAR0620
      DO 155 J#1,4                                                      SEAR0630
      TEM#X(J)                                                          SEAR0640
      IF(W(2,J)-TEM)148,150,150                                         SEAR0650
  148 W(2,J)#TEM                                                        SEAR0660
  150 IF(TEM-W(1,J))152,155,155                                         SEAR0670
  152 W(1,J)#TEM                                                        SEAR0680
  155 CONTINUE                                                          SEAR0690
      IF(KFUN-403)165,160,600                                           SEAR0700
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES MODEL BOX *****          SEAR0710
  160 DO 162 J#1,3                                                      SEAR0720
      DX(J)#0.                                                          SEAR0730
      DO 162 I#1,3                                                      SEAR0740
  162 DX(J)#DX(J)+ABSF(REFV(J,I)*AIN(I+4))                              SEAR0750
      GO TO 170                                                         SEAR0760
C     ***** FIND PARALLELEPIPED WHICH ENCLOSES DMAX SPHERE *****        SEAR0770
  165 T1#1.-A(4)*A(4)-A(5)*A(5)-A(6)*A(6)+2.*A(4)*A(5)*A(6)             SEAR0780
      DO 168 J#1,3                                                      SEAR0790
  168 DX(J)#SQRTF((1.-A(J+3)**2)/T1)*DMAX/A(J)                          SEAR0800
C     ***** START SEARCH AROUND REFERENCE ATOMS *****                   SEAR0810
  170 DO 500 ITOM#ITOM1,ITOM2                                           SEAR0820
      T1#FLOATF(ITOM)*100000.+SYITOM                                    SEAR0830
      CALL ATOM(T1,Y)                                                   SEAR0840
      IF(NG)171,172,171                                                 SEAR0850
  171 CALL ERPNT(T1,KFUN)                                               SEAR0860
      GO TO 500                                                         SEAR0870
C     ***** K#SYMMETRY EQUIVALENT POSITION *****                        SEAR0880
  172 NUM#0                                                             SEAR0890
  173 DO 400 K#1,NSYM                                                   SEAR0900
C     ***** SUBTRACT SYMMETRY TRANSLATION FROM REF ATOM *****           SEAR0910
      DO 175 J#1,3                                                      SEAR0920
  175 U(J)#Y(J)-TS(J,K)                                                 SEAR0930
C     ***** DETERMINE LIMITING CELLS TO BE SEARCHED *****               SEAR0940
C     ***** FIRST,MOVE THE BOX THROUGH THE SYMMETRY OPERATION *****     SEAR0950
      DO 185 J#1,3                                                      SEAR0960
      DO 185 L#1,2                                                      SEAR0970
      WW(L,J)#0.0                                                       SEAR0980
      DO 185 I#1,3                                                      SEAR0990
      TEM#FS(I,J,K)                                                     SEAR1000
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      IF(TEM)177,185,179                                                SEAR1010
  177 N#XMODF(L,2)+1                                                    SEAR1020
      GO TO 183                                                         SEAR1030
  179 N#L                                                               SEAR1040
  183 WW(L,J)#WW(L,J)+W(N,I)*TEM                                        SEAR1050
  185 CONTINUE                                                          SEAR1060
C     ***** CHECK FOR MIXED INDEX TRANSFORMATION *****                  SEAR1070
      DO 215 J#1,2                                                      SEAR1080
      TEM#FS(1,J,K)                                                     SEAR1090
      IF(TEM+FS(2,J,K))215,201,215                                      SEAR1100
  201 IF(TEM)203,215,207                                                SEAR1110
  203 WW(1,J)#W(2,4)*TEM                                                SEAR1120
      WW(2,J)#W(1,4)*TEM                                                SEAR1130
      GO TO 215                                                         SEAR1140
  207 WW(1,J)#W(1,4)*TEM                                                SEAR1150
      WW(2,J)#W(2,4)*TEM                                                SEAR1160
  215 CONTINUE                                                          SEAR1170
C     ***** MOVE 4 CELLS AWAY THEN MOVE BACK UNTIL PARALLELEPIPED AROUNDSEAR1180
C         REF ATOM AND BOX AROUND TRANSFORMED ASYM UNIT INTERSECT ***** SEAR1190
      N#0                                                               SEAR1200
      DO 235 J#1,3                                                      SEAR1210
      DO 225 I#1,2                                                      SEAR1220
      N#N+1                                                             SEAR1230
      TT#(U(J)-WW(I,J))*FLOATF(I*2-3)-DX(J)                             SEAR1240
      TEM#5.0                                                           SEAR1250
  221 TEM#TEM-1.0                                                       SEAR1260
      IF(TEM+TT)225,225,221                                             SEAR1270
  225 NW(N)#TEM*FLOATF(I*2-3)+5.                                        SEAR1280
C     ***** IF NO POSSIBILITY OF A HIT, GO TO NEXT SYMMETRY OPER *****  SEAR1290
      IF(NW(N)-NW(N-1))400,235,235                                      SEAR1300
  235 CONTINUE                                                          SEAR1310
C     ***** L CELL TRANSLATIONS IN X *****                              SEAR1320
      DO 395 L#LL,LU                                                    SEAR1330
      V(1)#U(1)+FLOATF(L-5)                                             SEAR1340
C     ***** M CELL TRANSLATIONS IN Y *****                              SEAR1350
      DO 395 M#ML,MU                                                    SEAR1360
      V(2)#U(2)+FLOATF(M-5)                                             SEAR1370
C     ***** N CELL TRANSLATIONS IN Z *****                              SEAR1380
      DO 395 NN#NL,NU                                                   SEAR1390
      V(3)#U(3)+FLOATF(NN-5)                                            SEAR1400
C     ***** I # TARGET ATOM *****                                       SEAR1410
      DO 395 I#ITAR1,ITAR2                                              SEAR1420
      DO 250 J#1,3                                                      SEAR1430
      TEM#0.0                                                           SEAR1440
      DO 245 II#1,3                                                     SEAR1450
  245 TEM#TEM+FS(II,J,K)*P(II,I)                                        SEAR1460
C     ***** SEE IF WITHIN PARALLELEPIPED*****                           SEAR1470
      TEM#TEM-V(J)                                                      SEAR1480
      IF(DX(J)-TEM)395,395,250                                          SEAR1490
  250 X(J)#TEM                                                          SEAR1500
      IF(KFUN-403)255,252,255                                           SEAR1510
C     ***** SEE IF WITHIN MODEL BOX *****                               SEAR1520
  252 CALL VM(X,AAREV,VI(2))                                            SEAR1530
      DO 253 J#2,4                                                      SEAR1540
      IF(AIN(J+3)-ABSF(VI(J)))395,253,253                               SEAR1550
  253 CONTINUE                                                          SEAR1560
      GO TO 277                                                         SEAR1570
C     ***** SEE IF WITHIN SPHERE *****                                  SEAR1580
  255 DSQ#VMV(X,AA,X)                                                   SEAR1590
      IF(DMX-DSQ)395,256,256                                            SEAR1600
  256 IF(DSQ-.0001)258,260,260                                          SEAR1610
  258 IF(KFUN-402)395,260,395                                           SEAR1620
C     ***** SELECT VECTORS ACCORDING TO CODES IF ANY *****              SEAR1630
  260 TEM#SQRTF(DSQ)                                                    SEAR1640
      IF(NCD)277,277,268                                                SEAR1650
  268 DO 275 J#1,NCD                                                    SEAR1660
  269 IF(ITOM-KD(1,J))275,270,270                                       SEAR1670
  270 IF(KD(2,J)-ITOM)275,271,271                                       SEAR1680
  271 IF(I-KD(3,J))   275,272,272                                       SEAR1690
  272 IF(KD(4,J)-I)   275,273,273                                       SEAR1700
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  273 IF(TEM-CD(1,J)) 275,274,274                                       SEAR1710
  274 IF(CD(2,J)-TEM) 275,277,277                                       SEAR1720
  275 CONTINUE                                                          SEAR1730
      GO TO 395                                                         SEAR1740
  277 VI(1) # 100000.*FLOATF(I)+FLOATF((1110-L*100-M*10-NN)*100+K)      SEAR1750
      IF(KFUN-402)278,325,325                                           SEAR1760
C     ***** DETERMINE CORRECT POSITION IN SORTED VECTOR TABLE *****     SEAR1770
  278 IF(NUM)317,317,279                                                SEAR1780
  279 DO 315 II#1,NUM                                                   SEAR1790
      TT#S(2,II)-TEM                                                    SEAR1800
      IF(ABSF(TT)-0.0001)297,297,281                                    SEAR1810
  281 IF(TT)315,297,283                                                 SEAR1820
C     ***** MOVE LONGER VECTORS TOWARD END OF TABLE *****               SEAR1830
  283 IF(200-NUM)287,287,289                                            SEAR1840
  287 NUM#199                                                           SEAR1850
  289 IJ#NUM                                                            SEAR1860
      DO 295 J#II,NUM                                                   SEAR1870
      S(1,IJ+1)#S(1,IJ)                                                 SEAR1880
      S(2,IJ+1)#S(2,IJ)                                                 SEAR1890
  295 IJ#IJ-1                                                           SEAR1900
      GO TO 319                                                         SEAR1910
C     ***** CHECK FOR DUPLICATE VECTORS IF DISTANCES ARE EQUAL *****    SEAR1920
  297 CALL ATOM(S(1,II),Z)                                              SEAR1930
      DO 305 J#1,3                                                      SEAR1940
      IF(ABSF(X(J)+Y(J)-Z(J))-0.0001)305,305,315                        SEAR1950
  305 CONTINUE                                                          SEAR1960
      GO TO 395                                                         SEAR1970
  315 CONTINUE                                                          SEAR1980
      IF(200-NUM)395,395,317                                            SEAR1990
C     ***** STORE THE RESULT IN VECTOR TABLE *****                      SEAR2000
  317 II#NUM+1                                                          SEAR2010
  319 NUM#NUM+1                                                         SEAR2020
      S(1,II)#VI(1)                                                     SEAR2030
      S(2,II)#TEM                                                       SEAR2040
      GO TO 395                                                         SEAR2050
C     ***** STORE RESULT IN ATOMS TABLE *****                           SEAR2060
  325 DO 330 J#1,3                                                      SEAR2070
  330 VI(J+1)#X(J)+Y(J)                                                 SEAR2080
      CALL STORE                                                        SEAR2090
  395 CONTINUE                                                          SEAR2100
  400 CONTINUE                                                          SEAR2110
C     ***** PRINT OUT DISTANCES *****                                   SEAR2120
  421 FORMAT(1H010X,20HVECTORS FROM ATOM  (I3,1H,I5,1H)6X,8HTO ATOMSI4, SEAR2130
     18H THROUGHI4)                                                     SEAR2140
      I0#SYITOM                                                         SEAR2150
      WRITE OUTPUT TAPE NOUT,421,ITOM,I0,ITAR1,ITAR2                    SEAR2160
      IF(NUM)500,500,423                                                SEAR2170
  423 DO 435 I#1,NUM                                                    SEAR2180
      T2#S(1,I)                                                         SEAR2190
      I1#T2/100000.                                                     SEAR2200
      I2#T2-FLOATF(I1)*100000.                                          SEAR2210
      CALL ATOM(T2,Z)                                                   SEAR2220
      IF(I-1)432,432,434                                                SEAR2230
  427 FORMAT(1H 13X,2(A6,1X),39X,1H(I3,1H,I5,1H)3F7.4,7X,3HD #F6.3)     SEAR2240
  429 FORMAT(1H 13X,2(A6,1X),2(3H  (I3,1H,I5,1H)3F7.4,3X)4X,3HD #F6.3)  SEAR2250
  432 WRITE OUTPUT TAPE NOUT,429,CHEM(ITOM),CHEM(I1),ITOM,I0,(Y(J),J#1,3SEAR2260
     1),I1,I2,(Z(J),J#1,3),S(2,I)                                       SEAR2270
      GO TO 435                                                         SEAR2280
  434 WRITE OUTPUT TAPE NOUT,427,CHEM(ITOM),CHEM(I1),I1,I2,(Z(J),J#1,3),SEAR2290
     1S(2,I)                                                            SEAR2300
  435 CONTINUE                                                          SEAR2310
C     ***** CALCULATE ANGLES ABOUT REF ATOM IF CODE IS 102 *****        SEAR2320
  437 IF(NJ2-2)500,451,451                                              SEAR2330
  441 FORMAT(1H010X,18HANGLES AROUND ATOMI5)                            SEAR2340
  451 WRITE OUTPUT TAPE NOUT,441,ITOM                                   SEAR2350
      L#NUM-1                                                           SEAR2360
      IF(L)500,500,457                                                  SEAR2370
  457 DO 465 I#1,L                                                      SEAR2380
      T2#S(1,I)                                                         SEAR2390
      T3#S(2,I)                                                         SEAR2400
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      I1#T2/100000.                                                     SEAR2410
      I2#T2-FLOATF(I1)*100000.                                          SEAR2420
      CALL ATOM(T2,X)                                                   SEAR2430
      CALL DIFV(X,Y,U)                                                  SEAR2440
      CALL MV(AA,U,V2)                                                  SEAR2450
      M#I+1                                                             SEAR2460
      DO 465 J#M,NUM                                                    SEAR2470
      T4#S(1,J)                                                         SEAR2480
      J1#T4/100000.                                                     SEAR2490
      J2#T4-FLOATF(J1)*100000.                                          SEAR2500
      CALL ATOM(T4,Z)                                                   SEAR2510
      CALL DIFV(Z,Y,V)                                                  SEAR2520
      F#ARCCOS(VV(V,V2)/(T3*S(2,J)))                                    SEAR2530
  460 FORMAT(1H 13X,3(A6,1X),7X,3(2H (I3,1H,I5,1H)),31X,F6.2)           SEAR2540
  465 WRITE OUTPUT TAPE NOUT,460,CHEM(I1),CHEM(ITOM),CHEM(J1),I1,I2,ITOMSEAR2550
     1,I0,J1,J2,F                                                       SEAR2560
  495 CONTINUE                                                          SEAR2570
  500 CONTINUE                                                          SEAR2580
  600 RETURN                                                            SEAR2590
      END                                                               SEAR2600
*LIST8
*LABEL
      SUBROUTINE SPARE(NJ)                                              SPAR0010
      COMMON NG                                                         SPAR0020
      NG#9                                                              SPAR0030
      RETURN                                                            SPAR0040
      END                                                               SPAR0050
*LIST8
*LABEL
      SUBROUTINE STORE                                                  STOR0010
C     ***** STORE IN OR REMOVE FROM ATOMS ARRAY *****                   STOR0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    STOR0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)STOR0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) STOR0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) STOR0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   STOR0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   STOR0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     STOR0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   STOR0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD STOR0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCAL1STOR0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   STOR0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                STOR0140
      IF(LATM)481,481,450                                               STOR0150
  450 IF(500-LATM)455,455,460                                           STOR0160
  455 IF(NJ2-10)490,490,460                                             STOR0170
  460 L#LATM                                                            STOR0180
C     ***** CHECK FOR POSITIONAL DUPLICATION *****                      STOR0190
      DO 480 K#1,L                                                      STOR0200
      DO 465 J#2,4                                                      STOR0210
      IF(ABSF(V1(J)-ATOMS(J,K))-0.001)465,465,480                       STOR0220
  465 CONTINUE                                                          STOR0230
      IF(NJ2-10)490,490,470                                             STOR0240
C     ***** ATOM REMOVAL BY TABLE PUSHDOWN *****                        STOR0250
  470 LATM#LATM-1                                                       STOR0260
      DO 475 I#K,LATM                                                   STOR0270
      DO 475 J#1,4                                                      STOR0280
  475 ATOMS(J,I)#ATOMS(J,I+1)                                           STOR0290
      GO TO 490                                                         STOR0300
  480 CONTINUE                                                          STOR0310
  481 IF(NJ2-10)482,490,490                                             STOR0320
C     ***** STORE ATOM *****                                            STOR0330
  482 IF(499-LATM)490,483,485                                           STOR0340
  483 NG#16                                                             STOR0350
      CALL ERPNT (V1(1),400)                                            STOR0360
  485 LATM#LATM+1                                                       STOR0370
      DO 486 J#1,4                                                      STOR0380
  486 ATOMS(J,LATM)#V1(J)                                               STOR0390
  490 RETURN                                                            STOR0400
      END                                                               STOR0410
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*LIST8
*LABEL
      SUBROUTINE TMM(X,Y,Z)                                             TMM 0010
C     ***** TRANSPOSE(TRANSPOSE(X)*Y)#Z *****                           TMM 0020
C     ***** X,Y,Z ARE 3X3 MATRICES *****                                TMM 0030
      DIMENSION X(3,3),Y(3,3),Z(3,3)                                    TMM 0040
      DO 115 I#1,3                                                      TMM 0050
      DO 115 K#1,3                                                      TMM 0060
  115 Z(K,I)#X(1,I)*Y(1,K)+X(2,I)*Y(2,K)+X(3,I)*Y(3,K)                  TMM 0070
      RETURN                                                            TMM 0080
      END                                                               TMM 0090
*LIST8
*LABEL
      SUBROUTINE UNIT(X,Z,ITYPE)                                        UNIT0010
      DIMENSION X(3),Y(3),Z(3)                                          UNIT0020
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    UNIT0030
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)UNIT0040
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) UNIT0050
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) UNIT0060
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   UNIT0070
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   UNIT0080
      DIMENSION XLNG(3),XO(3),XT(3)                                     UNIT0090
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   UNIT0100
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD UNIT0110
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIUNIT0120
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   UNIT0130
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                UNIT0140
      Y(1)#X(1)                                                         UNIT0150
      Y(2)#X(2)                                                         UNIT0160
      Y(3)#X(3)                                                         UNIT0170
      IF(ITYPE)125,125,105                                              UNIT0180
  105 TI#SQRTF(Y(1)*Y(1)+Y(2)*Y(2)+Y(3)*Y(3))                           UNIT0190
      GO TO 145                                                         UNIT0200
  125 TI#SQRTF(Y(1)*(Y(1)*AA(1,1)+Y(2)*(AA(1,2)+AA(2,1))+Y(3)*(AA(1,3)+AUNIT0210
     1A(3,1)))+Y(2)*(Y(2)*AA(2,2)+Y(3)*(AA(2,3)+AA(3,2)))+Y(3)*Y(3)*AA(3UNIT0220
     2,3))                                                              UNIT0230
  145 IF(TI)155,155,175                                                 UNIT0240
  155 NG#5                                                              UNIT0250
      GO TO 300                                                         UNIT0260
  175 Z(1)#Y(1)/TI                                                      UNIT0270
      Z(2)#Y(2)/TI                                                      UNIT0280
      Z(3)#Y(3)/TI                                                      UNIT0290
  300 RETURN                                                            UNIT0300
      END                                                               UNIT0310
*LIST8
*LABEL
      SUBROUTINE VM(X,Y,Z)                                              VM  0010
C     TRANSPOSED VECTOR TIMES MATRIX                                    VM  0020
C     Z(3)#X(3)*Y(3,3)                                                  VM  0030
      DIMENSIONX(3),Y(3,3),Z(3)                                         VM  0040
      DO115J#1,3                                                        VM  0050
      Z(J)#0.0                                                          VM  0060
      DO115I#1,3                                                        VM  0070
  115 Z(J)#Z(J)+X(I)*Y(I,J)                                             VM  0080
      RETURN                                                            VM  0090
      END                                                               VM  0100
*LIST8
*LABEL
      FUNCTION VMV(X1,Q,X2)                                             VMV 0010
C     TRANSPOSED VECTOR * MATRIX * VECTOR                               VMV 0020
C     VMV#X1(3)*Q(3,3)*X2(3)    TO  EVALUATE QUADRATIC OR BILINEAR FORM VMV 0030
      DIMENSION X1(3),Q(3,3),X2(3)                                      VMV 0040
      TI#0.                                                             VMV 0050
      DO 10 J#1,3                                                       VMV 0060
   10 TI#TI+X1(J)*(X2(1)*Q(J,1)+X2(2)*Q(J,2)+X2(3)*Q(J,3))              VMV 0070
      VMV#TI                                                            VMV 0080
      RETURN                                                            VMV 0090
      END                                                               VMV 0100
*LIST8
*LABEL
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      FUNCTION VV(X,Y)                                                  VV   0010
C     TRANSPOSED VECTOR * VECTOR                                        VV   0020
C     VV#X(3)*Y(3)                                                      VV   0030
      DIMENSIONX(3),Y(3)                                                VV   0040
      VV#X(1)*Y(1)+X(2)*Y(2)+X(3)*Y(3)                                  VV   0050
      RETURN                                                            VV   0060
      END                                                               VV   0070
*LIST8
*LABEL
      SUBROUTINE XYZ(QA,X,ITYPE)                                        XYZ 0010
C     ***** ITYPE .GT.0 CART. COORD. FROM ATOM CODE WORD *****          XYZ 0020
C     ***** XABSF(ITYPE) .LE.2 FOR WORKING SYSTEM *****                 XYZ 0030
C     ***** XABSF(ITYPE) .GT.2 FOR REFERENCE SYSTEM *****               XYZ 0040
C     ***** ITYPE .LE.0 USES TRICLINIC COORD. XT *****                  XYZ 0050
      DIMENSION X(3)                                                    XYZ 0060
      DIMENSION A(9),AA(3,3),AAREV(3,3),AAWRK(3,3),AID(3,3),AIN(140)    XYZ 0070
      DIMENSION ATOMS(4,500),BB(3,3),CD(8,20),CHEM(200),CONT(5),D(3,130)XYZ 0080
      DIMENSION DA(3,3),DP(2,130),EV(3,200),FS(3,3,48),KD(5,20),ORGN(3) XYZ 0090
      DIMENSION P(3,200),PA(3,3,200),PAC(3,5),PAT(3,3),Q(3,3),REFV(3,3) XYZ 0100
      DIMENSION RES(4),RMS(5),SYMB(3,3),TITLE(12),TITLE2(12),TS(3,48)   XYZ 0110
      DIMENSION VT(3,4),V1(4),V2(3),V3(3),V4(3),V5(3),V6(3),WRKV(3,3)   XYZ 0120
      DIMENSION XLNG(3),XO(3),XT(3)                                     XYZ 0130
      COMMON NG,A,AA,AAREV,AAWRK,AID,AIN,ATOMS,BB,BRDR,CD,CHEM,CONT,D   XYZ 0140
      COMMON DA,DP,DISP,EDGE,EV,FORE,FS,IN,ITILT,KD,LATM,LTNO,NATOM,NCD XYZ 0150
      COMMON NJ,NJ2,NOUT,NSR,NSYM,ORGN,P,PA,PAC,PAT,Q,REFV,RES,RMS,SCALIXYZ 0160
      COMMON SCAL2,SCL,SYMB,TAPER,THETA,TITLE,TITLE2,TS,VIEW,VT,V1,V2   XYZ 0170
      COMMON V3,V4,V5,V6,WRKV,XLNG,XO,XT                                XYZ 0180
      IT#XABSF(ITYPE)-2                                                 XYZ 0190
      NGI#NG                                                            XYZ 0200
      NG#0                                                              XYZ 0210
      IF(ITYPE)10,10,5                                                  XYZ 0220
    5 CALL ATOM(QA,XT)                                                  XYZ 0230
      IF(NG)30,10,30                                                    XYZ 0240
   10 T1#0.                                                             XYZ 0250
      DO 15 J#1,3                                                       XYZ 0260
      T2#XT(J)-ORGN(J)                                                  XYZ 0270
      V1(J)#T2                                                          XYZ 0280
   15 T1#T1+ABSF(T2)                                                    XYZ 0290
      IF(T1-.0001)20,20,40                                              XYZ 0300
   20 NG#NGI                                                            XYZ 0310
   30 DO 35 J#1,3                                                       XYZ 0320
   35 X(J)#0.                                                           XYZ 0330
      GO TO 300                                                         XYZ 0340
   40 IF(IT)45,45,60                                                    XYZ 0350
C     ***** RELATIVE TO WORKING SYSTEM *****                            XYZ 0360
   45 DO 55 I#1,3                                                       XYZ 0370
      T1#0.                                                             XYZ 0380
      DO 50 J#1,3                                                       XYZ 0390
   50 T1#T1+V1(J)*AAWRK(J,I)                                            XYZ 0400
   55 X(I)#T1*SCALI                                                     XYZ 0410
      GO TO 300                                                         XYZ 0420
C     ***** RELATIVE TO REFERENCE SYSTEM *****                          XYZ 0430
   60 DO 70 I#1,3                                                       XYZ 0440
      T1#0.                                                             XYZ 0450
      DO 65 J#1,3                                                       XYZ 0460
   65 T1#T1+V1(J)*AAREV(J,I)                                            XYZ 0470
   70 X(I)#T1*SCALI                                                     XYZ 0480
  300 RETURN                                                            XYZ 0490
      END                                                               XYZ 0500
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