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

Carroll K. Johnson

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

Carroll K. Johnson

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OAK RIDGE NATIONAL LABORATORY
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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																		
Dist. + ang.	0 or 2			101		ORG 1		ORG 2	TAR 1		TAR 2			D max (A)				
Princ. axes	0 or 2			102		ORG 1		ORG 2	TAR 1		TAR 2			D max (A)				
Dist. single convolute				103														
Dist. reiterate convolute				105		ORG 1		ORG 2	TAR 1		TAR 2			D max (A)				
Plotter control				106		ORG 1		ORG 2	TAR 1		TAR 2			D max (A)				
Initialize				201														
Advance and term.				202		X(IN)		Y(IN)										
Initialize CRT				203		XORG		YORG										
Change CRT intensity				204		12-IZORG												
Plot boundary																		
Dimensions				301		X(IN)		Y(IN)		VIEW(IN)		BRDR(IN)						
Title rotation				302		THE-TAT(")												
Retrace displace				303		X(IN)												
Atoms list																		
Run add				401		FROM (1)		() TO (1)	FROM (2)		() TO (2)		FROM (2)		() TO (3)			
Run subtract				411		FROM (1)		() TO (1)	FROM (2)		() TO (2)		FROM (2)		() TO (3)			
Sphere add	0 or 2			402		ORG 1		ORG 2	TAR 1		TAR 2		D max (A)					
Sphere subtract	0 or 2			412		ORG 1		ORG 2	TAR 1		TAR 2		D max (A)					
Box add				403		ORG 1		ORG 2	TAR 1		TAR 2		A/2 (A)		B/2 (A)		C/2 (A)	
Box subtract				413		ORG 1		ORG 2	TAR 1		TAR 2		A/2 (A)		B/2 (A)		C/2 (A)	
Triclinic box add				404		ORG 1		ORG 2	TAR 1		TAR 2		A/2		B/2		C/2	
Triclinic box subtract				414		ORG 1		ORG 2	TAR 1		TAR 2		A/2		B/2		C/2	
Convolute add				405		ORG 1		ORG 2	TAR 1		TAR 2		D max (A)					
Convolute subtract				415		ORG 1		ORG 2	TAR 1		TAR 2		D max (A)					
Reiterate convolute add				406		ORG 1		ORG 2	TAR 1		TAR 2		D max (A)					
Reiterate convolute subtr.				416		ORG 1		ORG 2	TAR 1		TAR 2		D max (A)					
Zero atoms list				410														
Cartesian system																		
Definition				501		ORGN		VIA	VIR		V2A		V2H					
Rotate reference				502		Axis No.		Rotate (")	Axis No.		Rotate (")							
Rotate working				503		Axis No.		Rotate (")										
Translate working				504		ΔX (IN)		ΔY (IN)										
Origin at centroid				505														
Inertial axis system and origin at centroid				506														
Store overlap data (Also see B.22, B.21)	0 or 2			511		$\begin{cases} 0 \\ 1 \end{cases}$ OVMRGIN (IN)												

Table 2.1 (continued)

Function	1 3	4 9	10 18	19 27	28 36	37 45	46 54	55 63	64 72
Center and scale									
Explicit		601	XO (IN)	YO (IN)	SCALE	SCALE			
Scale only		602	XO (IN)	YO (IN)		SCALE			
Center only		603			SCALE	SCALE			
Center and scale		604				SCALE			
I.P. and I.S. ^d		611	ΔXO (IN)	ΔYO (IN)	$\Delta SCALE$	SCALE			
I.P. and scale		612	ΔXO (IN)	ΔYO (IN)		SCALE			
I.S. and center		613			$\Delta SCALE$	SCALE			
Ellipsoids									
Shaded football (Format No. 1 trailer card)	0 or 1	701	AO (IN)	AI (IN)	ANR (1)	ANR (2)	SYM HGT	PAR-OFF ^b	PER-OFF ^c
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 (Format No. 1 trailer card)	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	SYM HGT	PAR-OFF ^b	PER-OFF ^c
As above except no printed output of individual coordinates	0 or 1	711	AO (IN)	AI (IN)	ANR (1)	ANR (2)			
	0 or 1	712	(same as 701)						
	0 or 1	713	(same as 701)						
	0 or 1	714	(same as 701)						
	0 or 1	715	(same as 705)						
Bonds									
Explicit (cont.)	1 or 2	801	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	...
Implicit fancy (Format No. 2 trailer card)	2	802							
Implicit line (Format No. 2 trailer card)	2	803							
As above except no printed output	2	811	(same as 801)						
	2	812	(same as 802)						
	2	813	(same as 803)						
Bond overlap explicit	1 or 2	821	FROM (1)	TO (1)	FROM (2)	TO (2)	FROM (3)	TO (3)	...
Bond overlap implicit	2	822							
Labels									
Chem. Symb.		901	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Reg. titles Format No. 3 title card	3	902	ATOM-1	(ATOM-2)	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Proj. Vect. title Format No. 3 title card	3	903	ATOM-1	ATOM-2	X Edge Reset	Y Edge Reset	HGT (IN)	PAR-OFF	PER-OFF
Vector title Format No. 3 title card	3	913	ATOM-1	ATOM-2			HGT (IN)	PAR-OFF	PER-OFF

Table 2.1 (continued)

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

^aI.P. and I.S. signifies increment position and increment scale.

^bPAR-OFF signifies parallel offset (in.).

^cPER-OFF signifies perpendicular offset (in.).

2.2 Programming a Nonstereoscopic Illustration for OR TEP

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

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

The major portions of the hidden line segments of atoms and bonds that are partially or totally behind other atoms and bonds may be omitted by using the overlap-elimination features of OR TEP-II. However, there are often areas where additional manual touch-up is needed. This can be accomplished by erasing or "whiting out" the remaining unwanted line segments. Even with stereo views, the features are more effective if overlap is taken care of, especially when "opaque" ellipsoids are used.

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

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

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

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

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

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

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

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

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

A triclinic box of enclosure can be described with a 404 instruction (see 3.3.5.4) to contain the desired atoms for the subject definition. The scaling and positioning of the subject to fill the drawing area may be accomplished automatically with a 604 instruction (see 3.3.7.1).

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

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

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

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

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

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

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

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

2.3 Programming a Stereoscopic Illustration for OR TEP

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

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

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

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

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

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

2.4 Drawing the Cubane Structure: An Example

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

The cell parameters are

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

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

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

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

2.4.1 Data Input for Cubane

2.4.1.1 Title Card (see 3.2.1). - FORMAT (12A6)

Card No.

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

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

(2) 5.34 5.34 5.34 72.26 72.26 72.26

2.4.1.3 Symmetry Cards (see 3.2.3)

FORMAT (11, F14.10, 3F3.0, 2(F15.10, 3F3.0))

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

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

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

⁶N. F. M. Henry and K. Lonsdale (eds.), *International Tables for X-Ray Crystallography*, vol. 1, Kynoch, Birmingham, 1962.

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

Card No.

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

2.4.1.4 Atomic Parameter Cards. -

Positional parameters (see 3.2.4.1): **FORMAT (A6, 3X, 5F9.6, F9.0)**

Thermal parameters (see 3.2.4.2): **FORMAT (11, F8.6, 5F9.6, F9.0)**

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

Card No.

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

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

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

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

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

In the card deck for this sample program, extensive use of Format No. 3 trailer cards (see 3.3.1.4) is made as a method of including a comment with an instruction. This convention is not mandatory, but it is a convenient method for annotating a program. This example uses a wide range of instructions in order to demonstrate them. As in the case with any programming system, there are many ways of doing any given problem. The Formats are described in Sect. 3.3.

2.4.2 Analysis of Structure (see 3.3.2). — These instructions are not connected with producing the figure. They are shown here just to demonstrate how they are used. A 101 instruction is used to obtain a tabulation of the atoms surrounding one atom or a series of several designated atoms. To obtain a list of all atoms (hydrogen and carbon atoms) out to a limit of (say) 3.6! A about the two carbons C1 and C2, one would use the following instruction. (The notation is explained in Sect. 3.3.2.)

Card No.

(19) 101 155501 2 1 4 3.61

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

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

(20) 102 155501 2 1 4 1.8

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

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

(21) 201

The two plot boundary dimensions can be equal for the present illustration since the cubane molecule is a cube. Suppose we use an 11- by 11-in. boundary and specify a 1.5-in. margin to give a total working area of 9 by 9 in. A 30-in. view distance might be reasonable to use in viewing a model of this size.

(22) 301 11 11 30 1.5

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

(23) 303 0

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

where the several parts designate:

- 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.

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

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

(27)	604	0	0	0	1.54
------	-----	---	---	---	------

(28)	503	2	2.7
------	-----	---	-----

Since the structure will be drawn twice, once for each eye, the "saved sequence" feature can be used to shorten the program. Note that the instructions between the start

Card No.

and stop instructions are both executed and saved the first time through. They can then be re-executed as many times as desired by using the "execute saved sequence" instruction 1103.

The 1101 instruction starts the saved sequence.

(29) 1101

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

(30) 2 511 0

(31) 0 1 4 1 4 4 0.9 1.6 .04

The ATOMS list currently contains all the atom designators for one cubane molecule. We want to draw the molecule in two separate steps so that the hydrogen and carbon atoms can be given different graphical representations. To draw the carbon atoms (ANR = 1.2), we will construct a special code that (a) draws the three principal-plane forward traces and the boundary-plane trace (NPLANE = 4), (b) omits the reverse sides of the principal planes (NDOT = 0), (c) draws the forward principal axes without additional shading (NLINE = 1), and (d) omits the reverse principal axes (NDASH = 0). In addition we want the chemical symbols to be drawn with letters 0.2-in. high (before projection) and displaced from the atomic center by 0.6 in. in the horizontal direction and 0.7 in. in the vertical direction.

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

(33) 0 0 0 1 2

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

Since the hydrogen atoms (ANR = 3, 4) are to be drawn with a standard model, the construction details will be taken care of automatically. We want chemical symbols 0.2 in. high and offset 0.35 in. horizontally and 0.4 in. vertically.

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

(35) 0 0 0 3 4

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

Card No.

(36) 2 812

(37) 0

$\frac{1}{(a)} \quad 4$	$\frac{1}{(b)} \quad 4$	$\frac{4}{(c)}$	$\frac{.9}{(d)} \quad 1.6$	$\frac{.04}{(e)}$
-------------------------	-------------------------	-----------------	----------------------------	-------------------

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 Å, which will cover all covalent bond distances, and

(e) the bond radius, is 0.04 Å.

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

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

(38) 906 155504 155503 0 0 .15 0 -.4

(39) 916 255504 155505 0 0 .15 0 -.4

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

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

(41) CUBANE

The saved sequence can now be terminated.

(42) 1102

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

(43) 202 9

The stereo rotation of -2.7° about axis 2 is now performed in preparation for the right-eye view. (Note that this rotation starts with the reference orientation, not the previous working orientation.)

(44) 503 2 -2.7

Card No.

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

(45) 1103

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

(46) 202 20

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

(47) 202 0

Finally we terminate the job and exit from the program.

(48) -1

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

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

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

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

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

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

Fig. 2.3 Polyhedral Representation of Prismatic Perovskite 9-Hydrate.

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

```

CUBANE E.A. FLEISCHER 1960 J.A.C.S. 82, 3009
5.30 5.30 5.30 72.26 72.26 72.26
0 1 0 0 0 0 1 0 0 0 0 0
0 0 0 1 0 0 1 0 0 0 0 0
0 0 1 0 0 0 0 1 0 0 0 0
0 -1 0 0 0 0 -1 0 0 0 0 0
0 0 0 -1 0 0 0 -1 0 0 0 0
0 0 -1 0 0 0 0 0 -1 0 0 0
C1 -.00100 -.00250 -.00500 -.00020 -.00020 -.00510 -.00706
C2 .00630 .00600 .00600 -.00030 -.00030 -.00030 .10706
B1 .10 .21000 .21000 .21000 .7
B2 .10 .21000 .21000 .21000 .7
ORIG 0 0 0
1 3 101 155501 2 1 0 3.61
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****
3 102 155501 2 1 0 1.0
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****
3 221
***** INITIALIZE MECHANICAL PLOTTED PACKAGE. 203 FOR CRT PACKAGE *****
3 301 11. 11. 30. 1.5
***** 11X11 BOUNDARY, ONE INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****
3 303
***** ELIMINATE ALL RETRACING *****
3 002 555501 5 1 0 3.2
***** ENCLOSED SURFACE OF RADIUS 3.2 A ABOUT BUNNY ATOM 5,555,01 *****
3 501 555501 255501 155501 255501 155502
***** ORIGIN ON BUNNY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****
3 502 2 25. 1 20.
***** ROTATE 25 DEGREES ABOUT Y, THEN 20 DEGREES ABOUT NEW X *****
3 000 0 0 1.50
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS *****
3 503 2 2.7

```

Line	Command	Address
3	STEREO DIRECTION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****	300
3	1101	390
*****	START SAVE SEQUENCE *****	400
2	511 0	410
3	1 0 1 0 0 0.9 1.6 .00	420
*****	STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULTE	430
1	715 0 0 1 0 .20 .60 .75	440
3	1 2	450
*****	READ CARBON ATOM ELLIPSOIDS, ATCH NUMBER RUN 1-2 *****	460
1	712 0 .20 .35 .40	470
3	3 4	480
*****	READ HYDROGEN ATOM SPHERES, ATCH NUMBER RUN 3-4 *****	490
2	012	500
3	1 0 1 0 0 0.9 1.6 .00	510
*****	TYPE 4 BOND .00 A READ MARGINS, ATCHS 1-4 TO MEANS 1-4, 0.9-1.6 A	520
3	906 155500 155503 0 C .15 0 -.00	530
*****	LABEL BOND 155500-155503 WITH REGULAR BOND DISTANCE LABEL *****	540
3	916 255500 155505 0 0 .15 0 -.00	550
*****	LABEL BOND 255500-155505 WITH PERSPECTIVE BOND DISTANCE LABEL *****	560
3	902 555501 0 0 1.0 .25 0 0	570
	CUTANE	580
3	1102	590
*****	END OF SAVE SEQUENCE *****	600
3	202 5.	610
*****	ADVANCE PLOTTER 9 INCHES ALONG X *****	620
3	503 2 -2.7	630
*****	STEREO DIRECTION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****	640
3	1103	650
*****	ELC-01E SAVE SEQUENCE FOR RIGHT EYE DRAWING *****	660
3	232 20.	670
*****	ADVANCE PLOTTER 20 INCHES *****	680
3	202	690
*****	ADD BURN IN SLOT TO MAGNETIC TAPE *****	700
	-1	710

2.4.5.2 Listing of Input Coeffs for Potassium Peroxy 9-Hydrox. -

[illegible]

```

C6      .23      .360      .P01      .189      7      EXAP0270
M1      .27      .654      .839      .193      7      EXAP0280
M2      .23      .850      .136      .297      7      EXAP0290
M3      .27      .873      .829      .369      7      EXAP0300
M4      .23      .692      .046      .526      7      EXAP0310
M5      .27      .997      .243      .111      7      EXAP0320
M6      .23      .967      .980      .572      7      EXAP0330
M7      .27      .376      .470      .002      7      EXAP0340
M8      .23      .493      .262      .886      7      EXAP0350
M9      .27      .404      .150      .124      7      EXAP0360
ORGN      .13      .250      .500      .400      7      EXAP0370
          .13      .000      .000      .000      7      EXAP0380
1      .03      .000      .000      .000      7      EXAP0390
3      102 155531 555531      1      20      3.55      EXAP0400
***** DISTANCES, ANGLES AND EDGES OF RE AND C COORDINATION POLYMER ***** EXAP0410
3      201      EXAP0420
***** INITIALIZE CALCOMP PLOT PACKAGE ***** EXAP0430
3      301      12      11      12      7.05      EXAP0440
***** 12-20-1.95 @ 2.3 IN. DIAMETER PICTURES, 12 IN. AWAY, DIRECT STEREO VIEW ***** EXAP0450
3      401 225531 -226631      EXAP0460
***** STORE UNIT CELL CORNERS FOR CELL OUTLINE ***** EXAP0470
3      474      21      21      1      5      .13      .52      .57 EXAP0480
***** STORE CENTRAL ATOMS OF POLYMER ***** EXAP0490
3      475      1      5      1      20      3.52      EXAP0500
***** COMPUTE SPHERE OF ENCLOSURE WITH EACH CENTRAL ATOM ***** EXAP0510
3      501 155531 215531 215631 2155501 2155631      EXAP0520
***** 9 AXES HORIZONTAL, C AXIS VERTICAL, VIEWED ALONG -A AXIS ***** EXAP0530
3      604      EXAP0540
***** AUTOMATIC SCALE AND POSITION ***** EXAP0550
3      573      2      3      EXAP0560
***** STEREO ROTATION FOR LEFT EYE VIEW ***** EXAP0570
3      1101      EXAP0580
***** START SAVED SEQUENCE ***** EXAP0590
1      714      EXAP0600
3      EXAP0610
***** DRAW ORBITAL ATOMS SELECTIVELY ***** EXAP0620
2      413      EXAP0630
2      22 22 22 22 1 9.0 11.3 .01      EXAP0640
2      22 22 22 22 1 15.0 16.0 .01      EXAP0650
2      1 11 5 11 2 2.5 2.9 .04 -1 1 1.0 1.9      EXAP0660
2      1 12 5 19 1 2.6 4.4 .02 -2 2 2.6 3.1      EXAP0670
2      1 22 17 23 1 2.6 4.7 .02 -3 3 2.7 3.52      EXAP0680
2      1 22 9 23 1 2.6 4.59 .02 -4 4 2.7 3.3      EXAP0690
3      7 23 7 23 1 2.6 4.6 .02 -5 5 2.7 3.2      EXAP0700
***** DRAW POLYMER AND CELL OUTLINE ***** EXAP0710
3      1102      EXAP0720
***** END SAVED SEQUENCE ***** EXAP0730
3      202      2.6      EXAP0740
***** ADVANCE PLOTTER FOR RIGHT EYE VIEW ***** EXAP0750
3      501      2      -3      EXAP0760
***** STEREO ROTATION FOR RIGHT EYE VIEW ***** EXAP0770
3      1173      EXAP0780
***** REPEAT SAVED SEQUENCE ***** EXAP0790
3      202      12      EXAP0800
***** ADVANCE PLOTTER 10 IN. ***** EXAP0810
3      202      EXAP0820
***** ADD DUMMY PLOT 1 STOP CALCOMP ON PLOT NO. 3 ***** EXAP0830
          -1      EXAP0840

```


2.4.5.3 Listing of Output from the Monitor Output Tape of the Computer. -

CUBANE E.B.FLEISCHER 1964 J.A.C.S. 86,3089

DIRECT CELL PARAMETERS

5.33999 5.33999 5.33999 C ALPHA BETA GAMMA
72.260 72.260 72.260
0.3046971 0.3046971 0.3046971

RECIPROCAL CELL PARAMETERS

0.202207 0.202207 0.202207 C₀ ALPHA₀ BETA₀ GAMMA₀
103.506 103.506 103.506
COSINE -0.23353940 -0.23353940 -0.23353940

STEREOTYPE TRANSFORMATIONS

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

NO. ATOM

NO.	X	Y	Z	B11	B22	B33	A12	A13	A23	TYPE
1	0.107110	0.195190	0.107060	0.041000	0.042500	0.045000	-0.004200	-0.014200	-0.005100	0.
2	0.115460	0.115460	0.115460	0.046000	0.046000	0.046000	-0.014300	-0.014300	-0.014300	0.
3	0.324600	0.346800	0.184800	0.100000	0.0	0.0	0.0	0.0	0.0	7.
4	0.210000	0.210000	0.210000	0.100000	0.0	0.0	0.0	0.0	0.0	7.
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.

NO. ATOM

NO.	X	Y	Z	BMSD 1	BMSD 2	BMSD 3
1	0.107110	0.195190	0.107060	0.208899	0.239056	0.253794
2	0.115460	0.115460	0.115460	0.203704	0.247732	0.247732
3	0.324600	0.346800	0.184800	0.100000	0.100000	0.100000
4	0.210000	0.210000	0.210000	0.100000	0.100000	0.100000
5	0.0	0.0	0.0	0.100000	0.100000	0.100000

CUBANE E.B.FELISCHER 1964 J.A.C.S. 86,3889

ORTHOGONAL REFERENCE VECTORS BASED ON CRYSTAL AXES

X VECTOR
Y VECTOR
Z VECTOR
0.1872659E 00 -0.5990902E-01 -0.4722328E-01
0.0 0.1966133E 00 -0.5722328E-01
0.0 0.0 0.2022068E 00

POST-FACTOR TRANSFORMATION MATRIX

0.5339994E 01 0.9536743E-06 0.9536743E-06
0.1627090E 01 0.5086074E 01 0.9536743E-06
0.1627090E 01 0.1107799E 01 0.4945430E 01

(((((INSTRUCTION 101)))))

0.1555010E 06 0.2000000E 01 0.1000000E 01 0.4000000E 01 0.3610000E 01 0.0 0.0

***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 Å *****

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

101 155501 255501 1 4 3.610 0.0 0.0

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

C1	M1	3.55504	-0.3246	0.3468	0.1008	D = 1.012
C1	C1	1.55505	-0.1071	0.1071	0.1952	D = 1.549
C1	C1	1.55504	-0.1952	0.1071	0.1071	D = 1.549
C1	C2	2.55504	0.1155	0.1155	0.1155	D = 1.552
C1	C1	1.55502	0.1071	-0.1071	0.1952	D = 2.103
C1	C1	1.55503	0.1952	0.1071	0.1071	D = 2.103
C1	C2	2.55504	-0.1155	0.1155	0.1155	D = 2.202
C1	M1	3.55506	-0.3468	0.1008	0.3246	D = 2.202
C1	M1	3.55505	-0.1008	0.3246	0.3468	D = 2.306
C1	M2	4.55501	0.2100	0.2100	0.2100	D = 2.376
C1	C1	1.55504	0.1071	-0.1952	0.1071	D = 2.677
C1	M1	3.55503	0.1008	0.3246	0.3468	D = 3.052
C1	M1	3.55503	0.3468	0.1008	0.3246	D = 3.069
C1	M2	4.55501	-0.2900	0.2100	0.2100	D = 3.077
C1	M2	4.56504	-0.2100	0.7900	0.2100	D = 3.086
C1	M2	4.55504	-0.2100	0.2100	0.2100	D = 3.175
C1	M1	3.55605	-0.1008	0.3246	0.6532	D = 3.200
C1	M1	3.45603	-0.6532	0.1008	0.6734	D = 3.204
C1	M1	3.46504	-0.6734	0.6532	0.1008	D = 3.300
C1	C2	2.55504	-0.1155	0.0045	0.1155	D = 3.609

VECTORS FROM ATOM (2,55501) TO ATOMS 1 THROUGH

C2	M1	4.55501	0.2100	0.2100	0.2100	D = 1.109
C2	C1	1.55501	-0.1071	0.1952	0.1071	D = 1.552
C2	C1	1.55502	0.1071	-0.1071	0.1952	D = 1.552
C2	C1	1.55503	0.1952	0.1071	0.1071	D = 1.552
C2	C1	1.55504	0.1071	-0.1952	0.1071	D = 2.202
C2	C1	1.55505	-0.1071	0.1071	0.1952	D = 2.202
C2	C1	1.55504	-0.1952	0.1071	0.1071	D = 2.202
C2	M1	3.55501	-0.2246	0.3468	0.1008	D = 2.273
C2	M1	3.55502	0.1008	0.3246	0.3468	D = 2.273
C2	M1	3.55503	0.3468	0.1008	0.3246	D = 2.273
C2	M2	2.55504	-0.1155	0.1155	0.1155	D = 2.710
C2	M1	3.55504	0.2246	0.3468	0.1008	D = 3.091
C2	M1	3.55505	-0.1008	0.3246	0.3468	D = 3.091
C2	M1	3.55506	-0.3468	0.1008	0.3246	D = 3.091
C2	M1	3.56504	0.2246	0.6532	0.1008	D = 3.101
C2	M1	3.55605	-0.1008	0.3246	0.6532	D = 3.101
C2	M1	3.65506	0.6532	0.1008	0.3246	D = 3.101
C2	C1	1.55504	0.1071	-0.0040	0.1071	D = 3.609
C2	C1	1.55605	-0.1071	0.1071	0.0040	D = 3.609
C2	C1	1.65506	0.0040	-0.1071	0.1071	D = 3.609

(((INSTRUCTION 102))))
 0.1555010E 04 0.2000000E 01 0.1000000E 01 0.4000000E 01 0.1799999E 01 0.0 0.0

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

CODE	FROM ATOMS (MIN MAX)	TO ATOMS (MIN MAX)	WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS A B C
102	155501	255501	1 4 1.800 0.0 0.0

VECTORS FROM ATOM		(1,55501)	TO ATOMS	1 THROUGH	4		
C1	H1	(1,55501)	-0.1871	0.1952	0.1071	(3,55501)	-0.3246 0.3468 0.1848 D = 1.012
C1	C1	(1,55501)	-0.1071	0.1071	0.1952	(1,55504)	-0.1071 0.1071-0.1952 D = 1.549
C1	C1	(1,55501)	-0.1952	0.1071	0.1071	(1,55504)	-0.1952-0.1071 0.1071 D = 1.549
C1	C2	(2,55501)	0.1155	0.1155	0.1155	(2,55501)	0.1155 0.1155 0.1155 D = 1.552

ANGLES AROUND ATOM		1					
H1	C1	C1	(3,55501)	(1,55501)	(1,55505)	D = 2.202	A = 124.69
H1	C1	C1	(3,55501)	(1,55501)	(1,55506)	D = 2.306	A = 127.16
H1	C1	C2	(3,55501)	(1,55501)	(2,55504)	D = 2.273	A = 123.92
C1	C1	C1	(1,55505)	(1,55501)	(1,55506)	D = 2.103	A = 89.40
C1	C1	C2	(1,55505)	(1,55501)	(2,55501)	D = 2.202	A = 90.40
C1	C1	C2	(1,55506)	(1,55501)	(2,55501)	D = 2.202	A = 90.40

VECTORS FROM ATOM		(2,55501)	TO ATOMS	1 THROUGH	4		
C2	H2	(2,55501)	0.1155	0.1155	0.1155	(4,55501)	0.2100 0.2100 0.2100 D = 1.109
C2	C1	(2,55501)	0.1071	0.1952	0.1071	(1,55504)	-0.1071 0.1952 0.1071 D = 1.552
C2	C1	(2,55501)	0.1071	0.1071	0.1952	(1,55502)	0.1071-0.1071 0.1952 D = 1.552
C2	C1	(2,55501)	0.1952	0.1071	0.1071	(1,55503)	0.1952 0.1071-0.1071 D = 1.552

ANGLES AROUND ATOM		2					
H2	C2	C1	(4,55501)	(2,55501)	(1,55501)	D = 2.376	A = 125.66
H2	C2	C1	(4,55501)	(2,55501)	(1,55502)	D = 2.376	A = 125.66
H2	C2	C1	(4,55501)	(2,55501)	(1,55503)	D = 2.376	A = 125.66
C1	C2	C1	(1,55501)	(2,55501)	(1,55502)	D = 2.103	A = 89.40
C1	C2	C1	(1,55501)	(2,55501)	(1,55503)	D = 2.103	A = 89.40
C1	C2	C1	(1,55502)	(2,55501)	(1,55503)	D = 2.103	A = 89.40

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

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

(((INSTRUCTION 301))))
 0.1100000E 02 0.1100000E 02 0.3000000E 02 0.1500000E 01 3.0 0.0 0.0

***** 11X11 BOUNDARY, 820 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****

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

```

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

===== ELIMINATE ALL RETRACING =====
RETRACE DISPLACEMENT = 0.0 INCH

(((( INSTRUCTION 402 ))))
0.3555010E 06 0.3000000E 01 0.1000000E 01 0.4000000E 01 0.3200000E 01 0.0 0.0

===== ENCLOSURE SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 =====

CODE FROM ATOMS TO ATOMS WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSIONS
402 55501 55501 1 4 3.200 0.0 0.0

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

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

(((( INSTRUCTION 501 ))))
0.5555010E 04 0.2555010E 04 0.1555010E 04 0.2555010E 06 0.1555020E 06 0.0 0.0

===== CRIGIN ON DUMMY ATOM 55501, VECTORS ALONG 2 EDGES OF CUBING =====
ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD. 0.0 0.0 0.0

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXIS
X VECTOR Y VECTOR Z VECTOR POST-PA:FOR TRANSFORMATION MATRIX
-0.1950173E 00 -0.5332411E-01 0.3517494E-02 -0.5161572E 01 2.2120971E 00 0.1354190E 01
0.5138092E-01 0.4031152E-02 0.1953263E 00 -0.1760902E 00 2.7350079E 01 0.5759129E 01
-0.5416121E-02 0.1950785E 00 -0.5144400E-01 -0.1402325E 01 0.5165090E 01 0.2624693E 00

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

===== ROTATE 25 DEGREES ABOUT Y, THEN 20 DEGREES ABOUT NEW Z =====
ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD. 0.0 0.0 0.0

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXIS
X VECTOR Y VECTOR Z VECTOR POST-PA:FOR TRANSFORMATION MATRIX
-0.1752591E 00 -0.6727112E-01 0.5055124E-01 -0.1065122E 01 -0.1411451E 01 0.3104037E 01
0.1292071E 00 -0.6943020E-01 0.1391012E 00 0.1930112E 01 -0.1037061E 01 0.4065206E 01
-0.2664603E-01 0.1934117E 00 0.5262519E-01 -0.1160019E 01 0.0153604E 01 0.3149157E 01

(((( INSTRUCTION 604 ))))
0.0 0.0 0.0 0.1500000E 01 0.0 0.0

===== AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS ==
ORIGIN POINT IN PLOTTER COORD. ( 5.35, 5.75 ) IN.
OVERALL SCALE = 1.940 INCH/ANGSTROM ELLIPSOID SCALE = 1.540
VIEW DISTANCE 30.000 INCHES

```

```

(((( INSTRUCTION 503 ))))
0.2000000E 01 0.2700000E 01 0.0 0.0 3.0 0.0 0.0

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

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD. 0.0 0.0 0.0

ORTHONORMAL WORKING VECTORS BASED ON CRYSTAL AXES
X VECTOR Y VECTOR Z VECTOR POST-FACTOR TRANSFORMATION MATRIX
-0.1726031E 00 -0.0727211E-01 0.5075099E-01 -0.3935544E 01 -0.1411451E 01 0.3200020E 01
0.1356199E 00 -0.6943020E-01 0.1329401E 00 0.2157155E 01 -0.1057061E 01 0.4760971E 01
-0.2413946E-01 0.1934117E 00 0.5382206E-01 -0.1010300E 01 0.4153644E 01 0.3200305E 01

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

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

(((( INSTRUCTION 511 ))))
0.0 0.0 0.0 0.0 3.0 0.0 0.0 0.0 0.0
1 4 1 4 4 0.90000 1.60000 0.04000 0.0 0.0 0.0 0.0 0.0

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

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

BOND SELECTION CODES
(SEQUENCE(A)) (SEQUENCE(B)) (BOND) (DISTANCES) ( BOND ) (PERSP.--LABELS) (NORMAL--LABELS) (DIGITS)
( MIN MAX ) ( MIN MAX ) (TYPE) (MIN MAX) (RADIUS) (HEIGHT OFFSET) (HEIGHT OFFSET) (NUMBER)
1 4 1 4 4 0.90 1.60 0.040 0.0 0.0 0.0 0.0 0.
FAULT NO = 14 455504. 800

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

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD. 0.0 0.0 0.0

ORTHONORMAL REFERENCE VECTORS BASED ON CRYSTAL AXES
X VECTOR Y VECTOR Z VECTOR POST-FACTOR TRANSFORMATION MATRIX
-0.1752591E 00 -0.0727211E-01 0.5055124E-01 -0.4106512E 01 -0.1411451E 01 0.3100037E 01
0.1292071E 00 -0.6943020E-01 0.1391012E 00 0.1930112E 01 -0.1057061E 01 0.4065296E 01
-0.2664003E-01 0.1934117E 00 0.5262519E-01 -0.1160014E 01 0.4153644E 01 0.3109157E 01

(((( INSTRUCTION 715 ))))
0.4000000E 01 0.0 0.1000000E 01 0.0 0.2000000E 00 0.6000000E 00 0.7000000E 00
0.0 0.0 0.1000000E 01 0.2000000E 01 3.0 0.0 0.0

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

```

```

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

***** [BAND HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4] *****

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

***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A
BOND SELECTION CODES
(SEQUENCE(A)) (SEQUENCE(B)) (BOND) (DISTANCE) ( BOND ) (PERSP.--LABELS) (NORMAL--LABELS) (DIGITS)
( MIN MAX ) ( MIN MAX ) (TYPE) (MIN MAX) (RADIUS) (HEIGHT OFFSET) (HEIGHT OFFSET) (NUMBER)
  1      4      1      4      4  0.90  1.60  0.040  0.0      0.0      0.0      0.0      0.
FAULT NO = 14 455504. 800

(((( INSTRUCTION 904 ))))
  0.1555040E 04  0.1555030E 04  0.0      0.0      0.1500000E 00  0.0      -0.4000000E 00

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

(((( INSTRUCTION 916 ))))
  0.2555040E 04  0.1555050E 04  0.0      0.0      0.1500000E 00  0.0      -0.4000000E 00

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

(((( INSTRUCTION 902 ))))
  0.3555010E 04  0.0      0.0      0.1000000E 01  0.2500000E 00  0.0      0.0

CUBANE

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

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

(((( INSTRUCTION 202 ))))
  0.9000000E 01  0.0      0.0      0.0      3.0      0.0      0.0

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

(((( INSTRUCTION 503 ))))
  0.2000000E 01 -0.2700000E 01  0.0      0.0      3.0      0.0      0.0

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

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD.      0.0      0.0      0.0

ORTHOGONAL WORKING VECTORS BASED ON CRYSTAL AXES
X VECTOR      Y VECTOR      Z VECTOR
-0.1774457E 00 -0.8727211E-01  0.4223930E-01      -0.4240361E 01 -3.1411451E 01  0.2911142E 01
  0.1225073E 00 -0.6945028E-01  0.1451131E 00      0.1690702E 01 -0.1057061E 01  0.4950014E 01
-0.2909743E-01  0.1934117E 00  0.5131147E-01      -0.1307071E 01  0.4153644E 01  0.3091016E 01

POST-FACTOR TRANSFORMATION MATRIX

```

```

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

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

(((( INSTRUCTION 511 )))))
0.0      0.0      0.0      0.0      3.0      0.0      0.0      0.0
1 4 1 4 4 0.30000 1.60000 0.04000 0.0 0.0 0.0 0.0 0.0

***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT
OVERLAP MARGIN IS 0.042 INCH

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

BOND SELECTION CODES
(SEQUENCE(A)) (SEQUENCE(B)) (BOND) (DISTANCE) (BOND) (PERSP.--LABELS) (NORMAL--LABELS) (DIGITS)
( MIN MAX ) ( MIN MAX ) (TYPE) (MIN MAX) (RADII) (HEIGHT OFFSET) (HEIGHT OFFSET) (NUMBER)
1 4 1 4 4 0.30 1.60 0.040 0.0 0.0 0.0 0.0 0.0 0.
FAULT ON = 14 455504. 300

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

ORIGIN FOR PROJECTION AXIS IN CRYSTAL COORD. 0.0 0.0 0.0

ORTHOGONAL REFERENCE VECTORS BASED ON CRYSTAL AXES POST-FACTOR TRANSFORMATION MATRIX
X VECTOR Y VECTOR Z VECTOR
-0.1752591E 00 -0.0727211E-01 0.5055124E-01 -0.4106512E 01 -0.1411451E 01 0.3104037E 01
0.1292071E 00 -0.6943428E-01 0.1391812E 00 0.1930112E 01 -0.1057061E 01 0.4865296E 01
-0.2644003E-01 0.1934117E 00 0.5262510E-01 -0.1160014E 01 0.4153444E 01 0.3149157E 01

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

***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****
(((( INSTRUCTION 712 )))))
0.0 0.0 0.0 0.0 0.2000000E 03 0.3500300E 00 0.4000000E 00
0.0 0.0 0.3000000E 01 0.4000000E 01 0.0 0.0 0.0

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

```

```

(((( INSTRUCTION 012 ))))
      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
      1 4 1 4 4 0.0000 1.40000 0.0000 0.0      0.0      0.0      0.0

```

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

BOND SELECTION CODES

```

(SEQUENCE(A)) (SEQUENCE(B)) (BOND) (DISTANCE) (BOND) (PERSP.--LABELS) (NORMAL--LABELS) (DIGITS)
( MIN MAX) ( MIN MAX) (TYPE) (MIN MAX) (RADIUS) (HEIGHT OFFSET) (HEIGHT OFFSET) (NUMBER)
1 4 1 4 4 0.90 1.60 0.040 0.0 0.0 0.0 0.0 0.
FAULT NO = 14 455500. 800

```

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

***** LABEL BOND 155504-155505 WITH REGULAR BOND DISTANCE LABEL *****

```
((((( INSTRUCTION 916 )))))
      0.2553040E 06  0.1553050E 06  0.0      0.0      0.1500000E 00  0.0      -0.4000000E 00
```

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

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

GRADE

((((INSTRUCTION 110J))))						
0.0	0.0	0.0	0.0	0.0	0.0	0.0

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

```

(((( INSTRUCTION 202 ))))
0.20000000E 02 0.0      0.0      0.0      0.0      0.0      0.0

```

***** ADVANCE PLOTTED 20 INCHES *****

(((INSTRUCTION 402))))

***** ADD DUMMY PLOT TO MAGNETIC TAPE *****

((((INSTRUCTION -1))))

3. DETAILED OPERATING INSTRUCTIONS

3.1 Definitions

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

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

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

where

AN = ATOM NUMBER ($0 \leq AN \leq NATOM - 1$) the sequential number of the atom in the input list of atoms in the asymmetric unit, which contains **NATOM** atoms. Atom zero is not in the input atom list but refers to the crystal origin point (0, 0, 0).

TA, TB, TC = crystal lattice translation digits along cell edges *a*, *b*, and *c*. Each digit in ADC can range from 1 to 9; consequently, it is possible to move up to ± 4 lattice translations in any direction from the origin cell 5,5,5.

SN = symmetry operator number ($0 \leq SN \leq NSYM - 1$) the numerical position of the symmetry operator in the input symmetry operator list which contains **NSYM** entries. Symmetry operator number zero is not in the input list but refers to an identity operator. However, the identity operation (corresponding to position *x*, *y*, *z*) must in general also be somewhere in the input symmetry operator list and is usually the first operator.

Example: An atom designation code of 347502 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 Å to 2.4 Å. The metal-to-oxygen vectors can be specified by the vector search code (1 2) (6 12) (1.9 2.4). Several variations of this basic code are used in the program.

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

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

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

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

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

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

3.1.9 Prime Parameters and Primer Constants. – In the process of mathematically describing an illustration to be machine drawn, many parameters must be used. The more basic among these parameters are called *Prime Parameters*. The values assigned to these prime parameters are often similar or identical from one problem to the next. The first thing OR TEP does is to call subroutine PRIME, which sets as many prime parameters as possible to reasonable, "in the ball park," *Primer Constants*. For example, the maximum plot dimensions (instruction 300 series) are set at 17.0 in. for x maximum and 11.0 in. for y maximum, and the overall scale for plotting (instruction 600 series) is set at 1.0 in. A. If the value assigned to a particular constant by the primer routine is satisfactory, the user does not have to reset this constant with OR TEP instructions.

3.2 Crystal Structure Data Input

3.2.1 Title Card. – FORMAT (12A6)

Columns

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

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

Columns	Type A	Type B	Type C	Type D
1–9	a (A)	a (A)	a* (A ⁻¹)	a* (A ⁻¹)
10–18	b (A)	b (A)	b* (A ⁻¹)	b* (A ⁻¹)
19–27	c (A)	c (A)	c* (A ⁻¹)	c* (A ⁻¹)
28–36	α (deg)	cos α	α^* (deg)	cos α^*
37–45	β (deg)	cos β	β^* (deg)	cos β^*
46–54	γ (deg)	cos γ	γ^* (deg)	cos γ^*

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

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

¹The routine assumes that a < 1.0 A, a* < 1.0 A⁻¹, α (or α^*) < 1.0°, and cos α (or cos α^*) < 1.0.

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

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 ≤ 5)	(b) Helix symmetry (70-72 ≤ 5)
1	/ 0 last card only	/ 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 symmetry³: Transformed triclinic coordinates (X_1, Y_1, Z_1) are obtained from input triclinic coordinates (X, Y, Z) by

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

or in matrix notation

$$X_1 = T + S X,$$

where

$T = (T_1, T_2, T_3)$ as fractions of cell edges.

(b) Helix screw symmetry:

$$X_1 = T + S X,$$

where

$T = (T_1, T_2, T_3 + L/N)$ as fractions of cell edge and

S a counterclockwise rotation of $L \cdot M \cdot N$ cycles about c^* axis.

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

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

³Only symmetry cards for general symmetry equivalent positions are permitted. Symmetry cards which explicitly designate special positions such as X, X, X ; X, X, Z ; $X, Y, 0$; $\frac{1}{2}, Y, 0$; and $\frac{1}{2}, \frac{1}{2}, 0$ are not allowed.

information or other information which specifies how the atom is to be represented on the drawing. The format allows the use of the atom parameter cards produced by the FORTRAN Least Squares Program OR FLS by Busing, Martin, and Levy (1962).⁴ Several alternate inputs are possible for each of the two cases, 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 / 0 for last atom only					
	Type 0,1,2,3,10	Type 4,5,8,9	Type 6		Type 7	
2-9	b_{11}	U_{11}	B	B	R	R
10-18	b_{22}	U_{22}	0	0	0	0
19-27	b_{33}	U_{33}	0	} VDC ₁	0	} VDC ₁
28-36	b_{12}	U_{12}	0		0	
37-45	b_{13}	U_{13}	0	} VDC ₂	0	} VDC ₂
46-54	b_{21}	U_{21}	0		0	
55-63	0,1,2,3,10	4,5,8,9	6 (or 0)	6 (or 0)	7	7

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

The coefficients b_{ij} ($i, j = 1, 2, 3$) of the anisotropic temperature factor, types 1, 2, 3, 10, are defined as follows: The complete temperature factor is

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

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

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

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

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

type 10: Base = e , $C = 2$, $D = 2^{-2}$.

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

$$\exp \left\{ -D(\sigma_1^2 U_{11}h^2 + \sigma_2^2 U_{22}k^2 + \sigma_3^2 U_{33}l^2 + C\sigma_1\sigma_2 U_{12}hk + C\sigma_1\sigma_3 U_{13}hl + C\sigma_2\sigma_3 U_{23}kl) \right\},$$

where σ_1^2 , σ_2^2 , σ_3^2 are reciprocal cell dimensions and in types 4 and 8, $C = 2$; in types 5 and 9, $C = 1$; in types 4 and 5, $D = 1$; in types 8 and 9, $D = 2^{-2}$. Type 6 allows the input of the Debye-Waller isotropic temperature factor B , which is used as follows:

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

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

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

When the isotropic temperature factor is used, the atom is represented as an isotropic ellipsoid (sphere) with equal principal axes of length μ . When the field in columns 19–27 is 0 or blank, the directions of the principal axes are along the standard Cartesian system axes (see 3.1.8). However, one can reorient these arbitrary orthogonal vectors by using the two vector designator codes VDC_1 and VDC_2 ; then the three new principal-axis vectors will be VDC_1 , $(VDC_1 \times VDC_2)$, and $VDC_2 \times (VDC_1 \times VDC_2)$. This is strictly an artistic feature of no physical significance.

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

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

3.3 Instruction Input

The instructions are the commands used in programming an illustration, and there is no required sequence for the instructions, except as indicated by the programming logic. Some instructions require

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

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

trailer cards, which may have three different formats. The program is informed what the format of the next card will be with the "look ahead" field, columns 1 to 3. The program action is also influenced by this information.

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

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

Columns

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

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

Columns

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

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

Table 3.1. Vector search code cards

Columns	Search instructions		Inertial axes		Bond plotting instructions			Negative No. in columns 43 to 48		
	101 402									
	102 412	505 506	801 811 821	802 812 822	803/813	802 812 822	803/813			
1-3	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead	Look ahead			
4-9	-	-	-	-	-	-	-			
10-12	} ORG. ANR	} ANR	-	} ANR (A)	} ANR (A)	} ANR (A)	} ANR (A)			
13-15			-							
16-18	} TAR. ANR	-	-	} ANR (B)	} ANR (B)	} ANR (B)	} ANR (B)			
19-21			-							
22-24	-	-	Bond type	Bond type	-	Bond type	-			
25-30	D min (A)	Weight	-	D min (A)	D min (A)	D min (A)	D min (A)			
31-36	D max (A)	-	-	D max (A)	D max (A)	D max (A)	D max (A)			
37-42	-	-	Bond radius (A)	Bond radius (A)	-	Bond radius (A)	-			
43-48	-	-	Perspective label hgt. (in.)	Perspective label hgt. (in.)	-	} ANR (P)	} ANR (P)			
49-54	-	-	Perpendicular displ. (in.)	Perpendicular displ. (in.)	-					
55-60	-	-	Nonperspective label hgt. (in.)	Nonperspective label hgt. (in.)	-	D _p min (A)	D _p min (A)			
61-66	-	-	Perpendicular displ. (in.)	Perpendicular displ. (in.)	-	D _p max (A)	D _p max (A)			
67-72	-	-	Digits indicator	Digits indicator	-	-	-			

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

Columns

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

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

3.3.2.1 Instructions 101 and 102. - These instructions call subroutine SEARCH, which finds all "target" atoms within a sphere of enclosure of radius $D_{\max}$ about a particular "origin" atom. The instruction card has an atom designator run (see 3.1.3) of origin atoms (Org. ADR) and an atom number run of target atoms (Tar. ANR). The Org. ADR allows one to calculate several spheres successively with a printout of results after each one. For example, suppose there are nine atoms in the input list and we want the total surroundings of atoms 365502, 465502, and 565502 out to a maximum radius, $D_{\max}$, of 4 Å. The Org. ADR is designated (365502, 5) or (365502, 565502)⁷ and the Tar. ANR is designated (1,9). Further selection of the interatomic vectors from a particular origin atom to the target atoms which fall within the limiting sphere is possible with vector search code (VSC) cards of Format No. 2 (see 3.3.1), which can be entered with the instruction. If VSC cards are present, then the vectors must also satisfy one of the VSC's in order to be saved. A VSC card to specify the selection of a shell of vectors in the above example might be coded as follows: Org. ADR (3,5) Tar. ANR (1,9) Dist. range (2.0, 2.7). More selective VSC's are also possible. They are meant to be based on known interatomic distance ranges, such as those tabulated in Vol. III of the *International Tables for X-Ray Crystallography*.⁸

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

⁷For the origin sequence 355501, 455501, 555501, an Org. ADR input (3,5) is allowed as well as (355501,5) and (355501,555501); however, the Tar. ANR must always be designated as shown. In sect. 2.1, Org. ADR is designated as ORG 1, ORG 2; and Tar. ANR is denoted by TAR 1, TAR 2. A minus sign preceding the second member of the Org. ADR is not required.

⁸H. Ondik and D. Smith, "Interatomic Distances in Inorganic Compounds," p. 257 in *International Tables for X-Ray Crystallography*, vol. III, ed. by K. Lonsdale, Kynoch, Birmingham, 1962.

The tabulation of atom designator codes, which is obtained automatically when these instructions are given, is often useful for planning an illustration. Although the tabulation is complete within the addressable region of 9^3 cells, the computing time is generally only a matter of seconds per sphere unless a very large D max is specified. Subroutine SEARCH is a rather elaborate routine designed to minimize computing time. This subroutine is also used for instructions 402 and 403, which are explained in 3.3.5.

Instruction card for instructions 101 and 102:

Columns

1-3	0 or 2 (look ahead)
4-9	101 or 102
10-18 } 19-27 }	Origin-ADR (atom designator run)
28-36 } 37-45 }	Target ANR (atom number run)
46-54	D max (A)

3.3.2.2 Instruction 103. – Principal axes of thermal motion (or arbitrary spheres, according to the temperature factor input) for all atoms in the input list are calculated. The printout contains root-mean-square amplitudes of displacement along the principal axes of the trivariate normal probability density function and direction cosines for the principal axes relative to the reference Cartesian base vectors. A symmetric covariance dispersion matrix based on the reference Cartesian system is also printed out. The diagonal elements are the mean-square displacements along the reference Cartesian axes.

Columns

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

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

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

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

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

Columns

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

3.3.3 Plotter Control Instructions (200 Series). – The 200 series is a group of instructions that control the plotter initialization, frame advance, termination, and any other peripheral commands that are required for a particular equipment configuration or plotting package. When the program is modified for a different equipment configuration, these series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements. Instructions for controlling the CalComp 765 and 835 off-line magnetic tape plotting systems⁹ are given here.

3.3.3.1 Instruction 201, Plot Package Initialization, Mechanical Plotter. – This instruction (or a 203 instruction) must be executed before any plotting can take place. It is a safe policy always to make this the first instruction card. It should be used only once per computer job regardless of how many plots are to be drawn during the job. If the 201 (203) and 301 instructions are omitted, all calculations are carried out but no plotting is done.

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

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

⁹The CalComp is an incremental plotter. The particular Benson-Lehner model available at Oak Ridge Central Data Processing Facility has also been used. The Benson-Lehner is an electromechanical x-y plotter with an analog converter. In general it seems that an incremental plotter is better suited to the requirement of OR TEP. The user should be warned that in the author's experience the magnetic tape plotting systems are notoriously troublesome; an annoying percentage of plot failures is to be expected because of equipment malfunctions. (This was true in 1965 and is still true in 1975.)

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

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

Columns

1-3 Blank

4-9 203

10-18 XORG } (new position of the origin of plotter coordinates relative to the lower left-hand corner of the normal CRT plotting area)

19-27 YORG }

28-36 IZORG (beam intensity origin)

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

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

Columns

1-3 Blank

4-9 204

10-18 $IZ - IZORG$

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

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

3.3.4.1 Instruction 301. — This instruction defines the limiting *x* and *y* dimensions, in inches, of the plot boundary and the border indentations. The boundary dimensions must not exceed those allowed by the plotter. The program will prevent the pen from getting closer than 0.1 in. to any boundary. The border indentation is an equal margin inside the entire boundary. When automatic scaling is used (600 series), the center points of the atoms are prevented from falling in the margin; but the atom represen-

ration, which has a finite size, may extend into that area. To compensate for the overlap, the border dimensions should be large when the overall drawing scale and the ellipsoid scale are expected to be large.

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

Columns		Primer Constant
1-3	-	-
4-9	301	-
10-18	Plot x limit (in inches)	17.
19-27	Plot y limit (in inches)	11.
28-36	View distance (in inches)	0. (parallel proj.)
37-45	Border (in inches)	0.5

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

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

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

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

3.3.5 Atom List Instructions (400 Series). – This series allows the user to specify which atoms are to be included in the illustration. The atom designators for the chosen atoms are stored in the ATOMS array for future use by other instructions. The ATOMS array can hold 500 atoms; but if the intended illustration has more than this, the illustration can be segmented and the segments drawn sequentially on the same plot.

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

3.3.5.1 Instructions #01 and #11, 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 #02 and #12, Sphere of Enclosure Add and Sphere of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete, partial, or vector screened, see 3.1.6) of a sphere of enclosure about any addressable point. For instruction 402, the contents of the spheres are *added* to the atom list except for positional duplications, which are omitted. In the 412 instructions, all points in the spheres are *eliminated* from the atoms list if they are present in that list. The instructions call subroutine SEARCH, and the instruction input details are identical to those of instructions 101 and 102 (see 3.3.2.1) except for the instruction number. In the monitor output, only the ATOMS list atom designator codes are printed and not the coordinates and interatomic distances. If the origin atoms on which the spheres of enclosure are centered are to be saved, the target atom number run (Tar. ANR) must contain this atom number. Furthermore, if vector search code cards of Format No. 2 are used, one of them must satisfy the intra-atom null vector for the origin atom in order to retain it.

3.3.5.3 Instructions 403 and 413, Box of Enclosure Add and Box of Enclosure Eliminate. – These instructions allow the user to build or modify the subject by specifying the contents (complete or partial but not vector screened, see 3.1.7) of a box of enclosure about any addressable point (or atom designator max 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, then a 501 or a 502 instruction, or both, should be used before this instruction to reorient the reference Cartesian system. After this instruction has been executed, the reference system can undergo further reorientation as desired for plotting purposes, etc.

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

Columns

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

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

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

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

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

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

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

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

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

3.3.6.1 Instruction 501, Reference Cartesian System Assignment. – Any Cartesian coordinate system is based on three orthonormal base vectors and an origin point. The origin point in the model (ORGN) is specified with an atom designator code. The three orthonormal base vectors can be described by two non-collinear vectors, and ORTEP 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)	$u \cdot v$	$(u \cdot v) \cdot u$
Base vector 3 (z axis)	$u \cdot (u \cdot v)$	$u \cdot v$

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

Columns		Effective Primer Constant
1-3	-	-
6-9	501	-
10-18	Origin (ADC)	000000
19-27	Vector u (VDC)	155501
28-36		165501
37-45	Vector v (VDC)	155501
46-54		156501
55-63	-	-
64-72	0 = Type A, >0 = Type B	1

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

Each operation requires two fields in the instruction card. For axial rotations, the first field of each pair will have the number 1, 2, or 3 to indicate rotation about the x , y , or z axes of the reference system. The second field will have the rotation angle in degrees for a right-handed rotation of the model about the designated axis (i.e., a positive angle signifies a counterclockwise rotation of the structure with the designated axis pointing toward the reader). The body diagonal rotation is designated by either a (-1) or a (-2) in the first field to indicate a 120° or a 240° right-handed rotation about the body diagonal, and the second field is blank. A (-3) would rotate the structure completely around and thus not change its previous orientation.

Columns

First Card

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

Second Card

10-18	ϕ_4
.	.
.	.
.	.

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

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

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

Columns

1-3	-
4-9	503
10-18	1,2,3
19-27	..

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

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

¹¹R. G. Saunders, *Appl. Opt.* **7**, 1499 (1968).

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

Columns

1-3 Blank

4-9 504

10-18 Translation of origin along x axis of reference system (in.)

19-27 Translation of origin along y axis of reference system (in.)

28-36 Translation of origin along z axis of reference system (in.)

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

503 2 2.45

and

503 2 -2.45 ,

are replaced by the stereo translation instructions

504 -1.28 0 0

and

504 2.56 0 0 ,

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

504 -1.28 0 0 .

in order to prevent confusion.

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

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

ORNL-DWG. 69-7541

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

ORNL DWG. 69-8122

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

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

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

3.3.7 Positioning and Scaling Instructions (600 Series). – These instructions are used to direct the placement of the origin point ORGN (specified by instruction 501) onto the drawing (dimensioned by instruction 301). In addition the three-dimensional assembly of atoms (chosen by the 400 series instruction) constituting the model is scaled. The atomic centers of the model will then be hanging in space above and below the drawing board correctly positioned to be projected from the eye point described with 301.

3.3.7.1 Normal Modes of Positioning and Scaling. – Several normal modes of operation are available to the user for positioning and scaling the model. Instruction 601 requires the user to supply a complete explicit description of position (x_0, y_0) and scale (SCAL1). At the other extreme, instruction 604 automatically scales and positions the model so that the peripheral projected atom centers will touch two

opposite borders and the peripheral atoms in the remaining dimensions will be centered on the drawing. An intermediate mode is available through 602, which provides automatic scaling after explicit positioning. In general this allows only one edge of the model to touch a border. Finally, instruction 603 requires an explicit scale and does automatic centering.

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

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

Columns	601	602	603	604	Primer Constant
1-3	-	-	-	-	-
4-9	601	602	603	604	-
10-18	x_0	x_0	-	-	8.5
19-27	y_0	y_0	-	-	5.5
28-36	SCAL1	-	SCAL1	-	1.0
37-45	SCAL2	SCAL2	SCAL2	SCAL2	1.54

3.3.7.2 Incremental Modes of Positioning and Scaling. - Additional flexibility is provided through the incremental instructions 611, 612, and 613. These allow the user to "nudge" the model or modify the scale factor (SCAL1), or both, after the parameters have been initially set with a previous 600 series instruction. The 611 instruction adds Δx_0 , Δy_0 to the previous x_0 , y_0 position for the ORGN placement and multiplies the existing SCAL1 by WK (except if WK = 0, SCAL1 is unmodified). Instruction 612 increments the position and then does an automatic scaling; 613 first increments the scale (by multiplying by WK) 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 WK = 0.9. This will simply reduce the scale 10% so that there is more space for labels, etc.

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

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

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

Figure 3.3 shows various combinations of these elements. It is obvious that certain of these combinations are better representations than others. Instruction 701 generates the 5A model of Fig. 3.3, instruction 702 generates 2A, and 703 produces 3B. Instruction 704 draws the boundary ellipse alone. If an atom is entered as a sphere, the boundary will be circular before projection and slightly elliptical after perspective projection. Instruction 705 allows the user to make up any representation from the basic components.

Chemical symbols up to six alphanumeric characters in length are included with the input structural parameters for each atom. These symbols can be put onto the illustration with one 700 series or several 900 series instructions. The 700 series places the center of the six-character field of each atom in the same position relative to the atom center; the 900 series allows the user to position each symbol individually. The 700 series requires only three parameters as follows: (1) symbol height in inches, (2) parallel (left-right) offset in inches, and (3) perpendicular (up-down) offset in inches. The parameters refer to the model before projection, and they will change slightly during perspective projection. The parallel and

Fig. 2.2. Various Combinations of Ellipsoid Components.

perpendicular offset refer to the exact center of the six-character input field and are relative to the lettering base line set up with the 302 theta rotation. A symbol height of 0 or blank will cause the symbol-drawing routine to be bypassed.

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

It is possible to vary the thickness of the boundary ellipse line by making it a function of z , the height of the atom from the drawing board. This option is normally used with the 704 (boundary only) instruction but will work for any 700 instruction. Entries are put in the A_0 and A_1 fields of the instruction continuation card to specify the coefficients of

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

where

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

A_0 is ΔR for an atom at $z = 0$, and

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

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

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

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

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

1. x, y plotter coordinates: the coordinates, in inches, for the projected atom center on the plot, measured from the lower left-hand corner of the limiting boundary. This is the fixed plotter coordinate system with origin point set by the plotter operator.
2. x, y, z working Cartesian coordinates: the coordinates, in inches, for the oriented and scaled atomic model before projection. The x and y axes parallel the plotter x and y axes, and the origin of the system is in the plane of the plotter at the point x_0, y_0 (see 3.3.7) in plotter coordinates. The point ORGN of the scaled model is at this point (see 3.3.6.1).
3. x, y, z triclinic coordinates, in fractions of the unit-cell edges relative to the crystal unit-cell origin.
4. Principal axes of thermal motion, consisting of (a) principal values of root-mean-square displacement and (b) direction cosine for principal vectors relative to the working Cartesian system.
5. The atom designator code and chemical symbol for the atom.

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

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

Columns

First Card

1-3	1 (if boundary retracing or atom selection is desired; otherwise 0)
4-9	701, 702, 703, 704, 711, 712, 713, 714
10-45	Blank
46-54	Symbol height (in.)
55-63	Parallel offset (in.)
64-72	Perpendicular offset (in.)

Second Card (needed only for boundary retracing or atom selection)

1-3	Blank
4-9	Blank
10-18	A_0 (in.) or blank
19-27	A_1 (in.) or blank
28-36	} ANR or blank
37-45	

3.3.8.2 Atom Plotting Instructions 705 and 715. -

Columns

First Card

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

} for symbols

Second Card same as 701

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

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

The more elaborate bond is the stick bond, which could also be called a conical bond because of its accentuated perspective taper.¹² Each end of the bond intersects either (1) an ellipsoid or (2) an enveloping cone (tangent cone) which has its apex at the viewpoint and is tangent to an ellipsoid. In general, the ellipsoid intersection is automatically used if the axis of the bond intersects the ellipsoid at a point which is visible to the viewpoint; otherwise, the tangent cone intersection is used, so that the bond appears to terminate at the boundary of the ellipsoid. However, the user can specify that the ellipsoid intersection always be used in order to make the skeleton type model (e.g., 3B of Fig. 3.1) appear even more transparent. The radius of the stick bond and the number of lines which are used to draw the bond are specified by input parameters.

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

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

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

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

2. The bond radius (mean value for stick bonds) is in Angstrom units. Values between 0.01 and 0.06 Å usually give good results. Any positive value may be used as long as it is smaller than the scaled ellipsoid minimum semidimension. The bond radius is not changed by the ellipsoid scale factor ratio SCAL2. The bond radius should not be made "vanishingly small" (e.g., $r < 0.005$ Å) if the overlap feature is used because numerical rounding may cause incorrect hidden-line elimination.

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

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

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

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

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

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

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

3.3.9.1 Instructions 801 and 811. Explicit Stick Bonds. — The bonds are described with two atom designator codes for each bond. The atom designator codes go on the 801 card and on Format No. 1 trailer cards (see Table 2.1 for format). The two atom designator codes for a bond must be in adjacent fields, but blank fields can be inserted between the different bonds. Since there are seven fields available per card, it is a good idea to use only two, four, or six of them so that the card sequence within the instruction (other than first and last cards) will be unimportant. In addition, a Format No. 2 trailer card is required with the fields specified under column 801 in Table 3.1 properly filled in.

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

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

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

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

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

General titles and bond length labels can be drawn either in perspective or parallel to the plane of the drawing. Chemical symbols and centered symbols are always drawn parallel to the plotter plane. Instructions 913 through 916 are for perspective lettering, and instructions 901 through 909 produce regular lettering.

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

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

The format for the entire 900 series is as follows:

Columns

1-3	Blank or 3 (or 1 if second card is needed)
4-9	Instruction number
10-18	Designator for atom A
19-27	Designator for atom B (or blank)
28-36	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 SYMBOL routine (the misspelling of "symbol" is intentional). The symbol number must be in the range 0-14.

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

The three instructions in this series are to start the saved sequence (instruction 1101), terminate the saved sequence (instruction 1102), and execute the saved sequence (instruction 1103). All instruction

cards and their trailer cards between the 1101 and 1102 instructions are executed and saved on a magnetic scratch tape. A 1103 instruction rewinds this scratch tape and repeats all the instructions stored there before another instruction is read from the monitor input. There are no parameters to be entered with the 1100 series instructions.

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

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

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

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

Columns

1-3 Blank

4-9 1201

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

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

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

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

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

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

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

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

Columns

1-3	2 (if bonds are to be stored, otherwise 0)
4-9	511
10-18	<div style="display: inline-block; vertical-align: middle; font-size: 3em; line-height: 1;">{</div> <div style="display: inline-block; vertical-align: middle;"> Blank or 0 - overlap margin default option described above 1 (or -1) - overlap margin = 0.0 0 OVERGN 1.0 - overlap margin OVERGN (in inches) </div>

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

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

3.3.1.4.3 Instruction 822. Implicit Bond Outline Storage. - Normally the information on implicit bond outlines is stored with the 511 card; however, if more than 10 Format No. 2 trailer cards are needed, the extra ones can be entered with this instruction. All ~~parameter~~ ~~cards~~ are entered with the Format No. 2 trailer cards (see Table 3.1). The only entry on the instruction card is the 2 in column 5 and 822 in columns 7-9.

3.4 List of Fault Indicators

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

NG	Subroutine Involved	Fault	Action
1	PRELIN	No sentinel found after reading 48 symmetry cards	Tries to read parameter cards
2	PRELIN	No sentinel found after reading the parameter cards for 100 atoms	Tries to read instruction cards
3	PRELIN	Anisotropic temperature factor coefficients form a matrix which is not positive definite	EXIT after printing out all principal values (imaginary ones are listed negative)
4	ATOM,PAXES	Symmetry operation number is higher than the number of input operations	Omit atom
5	ATOM,PAXES	Atom number is higher than the number of input atoms	Omit atom
6	EIGEN	Null temperature factor matrix or failure in bisection routine	EXIT, after printing out all principal values
7	EIGEN	Eigenvector routine failure due to null vector	EXIT, after printing out all principal values
9	MAIN,SPARE	Unidentified instruction number	Omit faulty instruction
10	BOND,F700	Atom out of bounds	Omit atom
11	F800	No vector search codes	Omit instruction
12	F600, SEARCH	Insufficient number of atoms in ATOMS list	EXIT
13	BOND	Imaginary bond intersection (i.e., bond larger than atom)	Omit bond
14	BOND	Hidden (end-on) bond	Omit bond
15	F900	Null vector as base line	Omit label
16	STORE	ATOMS list is full	Omit all succeeding atoms

4. COMPUTATIONAL PROCEDURES (HOW THE PROGRAM WORKS)

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

4.1 Graphic-Computational Methods

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

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

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

The basic algorithm for finding the points along a given general ellipse utilizes the properties of conjugate diameters. Assume that we have the three principal axis vectors $V1$, $V2$, $V3$ 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

$$V5 = AV4, \quad (4.1.1.1)$$

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

$$X^TAX = d, \quad (4.1.1.2)$$

where d is a constant.

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

$$V7 = V5 \times AV6. \quad (4.1.1.3)$$

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

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

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

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

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

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

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 V_1 and V_2 will have the third principal axis vector V_3 normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector V_8 where

$$V_8 = V_5 \times V_3. \quad (4.1.1.4)$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to V_8 and in the principal plane containing V_1 and V_2 is V_9 , where

$$V_9 = V_3 \times A V_8. \quad (4.1.1.5)$$

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

$$s = |d/(I^T A I)|^{1/2}. \quad (4.1.1.6)$$

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

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

where i is the cycle number.

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

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

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

The ellipsoid is described in matrix notation as

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

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

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

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

where

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

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

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

1. Form a radial set of vectors $\mathbf{V}_r$ of length r normal to $\mathbf{V}_b$.

2. Take a unit vector l parallel to V_0 and let

$$X_i = V_i + s l, \quad (4.1.2.4)$$

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

$$s^2 l^T A l + 2s V_0^T A l + V_0^T A V_0 - d = 0; \quad (4.1.2.5)$$

solving for s we get

$$s = \frac{-V_0^T A l + \sqrt{(V_0^T A l)^2 - (l^T A l)(V_0^T A V_0 - d)}}{l^T A l}. \quad (4.1.2.6)$$

The elliptic cone which is tangent to the ellipsoid and which has its apex on the viewpoint can be obtained from the matrix A and from the vector V_0 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 V_0 .
2. The tangent cone can now be described as

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

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

$$C = \begin{pmatrix} a_{11} + \frac{a_{13}a_{31}}{K-a_{33}} & a_{12} + \frac{a_{13}a_{32}}{K-a_{33}} & \frac{Ka_{13}}{K-a_{33}} \\ a_{21} + \frac{a_{23}a_{31}}{K-a_{33}} & a_{22} + \frac{a_{23}a_{32}}{K-a_{33}} & \frac{Ka_{23}}{K-a_{33}} \\ \frac{Ka_{31}}{K-a_{33}} & \frac{Ka_{32}}{K-a_{33}} & \frac{Ka_{33}}{K-a_{33}} \end{pmatrix}, \quad K = d/(V_0^T V_0). \quad (4.1.2.8)$$

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

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

$$Y = V_p + s l \quad (4.1.2.9)$$

and obtain from (4.1.2.7)

$$(V_p + s l)^T C (V_p + s l) = 0;$$

then solving for s we obtain

$$s = \frac{-V_p^T C I + \sqrt{(V_p^T C I)^2 - (I^T C I)(V_p^T C V_p)}}{I^T C I} \quad (4.1.2.10)$$

The vector V_p from the vertex to p is formed by

$$V_p = -V_0 + V_r,$$

where V_r is any member of a radial set such as that described for the regular ellipsoid intersection.

4.2 OR TEP Subprograms

The subprograms can be grouped into four functional categories. The first 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 "nursmaid routine" which is controlled through the 200 series instructions. It satisfies the whims and fancies of any particular plotting system control package.

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

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

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

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

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

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

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

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

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

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

4.2.2.3 DRAW (W,DX,DY,NPEN), DIMENSION W(3). – **DRAW** interconnects **OR TEP** and the plot package. It also prevents the pen from crossing the boundaries. If the indicator **ITILT** in common is zero, the array **W** contains **x** and **y** in plotter coordinates. While perspective lettering is being plotted, **ITILT** $\neq$ 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,NST). – This is the printout routine called when a Fault is found. The arguments identify the atom designator code and the instruction involved in the Fault. The fault indicator, **NG**, is in common.

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

ITYPE = 0 for covariance matrix

ITYPE = 0 for ellipsoid quadratic form matrix

ITYPE = 1 based on triclinic system

ITYPE = 2 based on working Cartesian system

ITYPE = 3 based on reference Cartesian system

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

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

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

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

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

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

ITYPE = 0: triclinic coordinates

ITYPE = 1 or 2: working Cartesian system coordinates

ITYPE = 3: reference Cartesian system coordinates

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

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

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

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

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

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

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

4.2.3.2 AXEQB (A,X,B,N), DIMENSION A(3,3),X(3,3),B(3,3). — This routine solves the matrix equation $A X = B$ 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: $A_1 = X$; $A_2 = (X \times Y)$; $A_3 = X \times (X \times Y)$

|ITYPE| = 2: $A_1 = X$; $A_2 = (X \times Y) \times X$; $A_3 = X \times Y$

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 (,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 $X \times Y$.

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 $(A^T B)^T = C$. 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 $X^T A = Y^T$. 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 $X^T A Y = \text{scalar}$.

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

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

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

a) **ENTRY – PLOTS (A, LENGTH, LTNO)**

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

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

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

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

In subroutine F200 we have

DIMENSION PLA(1500)

and card F2000180 contains

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

for the CDC 1604-A or

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

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

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

An ORTEP 201 instruction directs the execution of this initialization.

b) ENTRY - PLOT (X,Y,IPEN)

This is the basic entry to convey data to the subroutine for plotting. To facilitate the substitution of other plotting routines, ORTEP contains only one instruction (card DRAW0330 in subroutine DRAW) which calls this entry point. All the plotting information passes through DRAW before going to the actual plotting routine PLOT.

X is the abscissa expressed in inches.

Y is the ordinate expressed in inches.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

2. ENTRY - SIMBOL (X(1),X(2),H,NUM,THETA,L), DIMENSION X(3) (note $L \geq 0$)

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

H is the height of the symbol to be plotted.

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

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

THETA is the angle of rotation as described previously.

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

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

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

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

ENTRY - NUMBUR(X(1),X(2),H,A,THETA,N)

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

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

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

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

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

4.3 Adapting OR TEP to Other Equipment Configurations

Card images² for OR TEP will be provided to crystallographers and others who request that the program be sent to them.

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

²The size of the card deck (3000-6000 cards) is such that it is generally more economical to send the program on magnetic tape. If convenient, the user should send a blank magnetic tape to the author. Card images will be written on that tape in an agreed upon format and the tape returned to the sender.

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

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

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

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

1. Remove the "REAL*8 CHEN" card from the subprograms which use common.
2. Add the correct IBSYS monitor control cards including "SPOOL" and "SGROUP" cards to conserve memory space.

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

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

4.3.2 External Device Logical Number Assignments. - Logical device number assignments are made in subroutine **PRIME**. Four cards are involved in this initialization:

Magnetic Tape Function	Symbolic Name	Primer Constant	Location in PRIME
a) Monitor Input	IN	5	PRIM0220
b) Monitor Output	NOUT	6	PRIM0280
c) Scratch	NSR	8	PRIM0290
d) Plotting	LTNO	23	(PRIM0250)*

4.3.3 Plotter Systems Other than the CalComp 500. - In general, only subroutine **PLOTS** (with entries **PLOTS** and **PLOT**) needs to be replaced when a different plotting system is used. This routine is called from only two locations, one in F200 and the other in DRAW. F200 will probably have to be rewritten, and

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

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

Location DRAW9330 in subroutine DRAW should also be modified to call the new line-drawing routine with the correct argument.

4.3.4 Computing Systems Other Than the IBM 360, IBM 7090, and CDC 1604-A. - Basically, the ORTEP system is designed to be used on a 32 K memory. Consequently, ORTEP would have to be changed considerably to operate in a much smaller memory.

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

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

SUBCOL is called from BOND6460, BOND0480, F7060850, F9601310, F90C1340, and F9001470.

NUMBUR is called from BOND 2510 and F9001440.

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

4.4 Addition of New ORTEP Instructions

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

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

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

4.5 Glossary of Symbols in ORTEP Common, with Array Dimensions

	A(9)	Direct crystal cell parameters. $a, b, c, \cos \alpha, \cos \beta, \cos \gamma, \alpha, \beta, \gamma$.
	AA(3,3)	Metric tensor g where $g_{ij} = a_i \cdot a_j$.
	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 ORTEP instruction.
	ATOMS(4,500)	Column 1 contains atom designator code for the atoms which are to be included in the scaling, plotting, bond lengthing, 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 = AA ⁻¹ .
P	BRDR	Border width in inches extending inward from plot boundary.
	CD(8,10)	Part of vector search code array. Used in conjunction with KD array.
	CHEM(100)	Chemical symbols for the input atoms.
P	CONT(5)	Constants used in subroutine RADIAL.
	DI(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 PLTX.
	EV(3,100)	Root-mean-square displacements for each principal axis of each input atom.
P	FORE	Cosine of critical angle between bond and Cartesian z axis vectors for perspective bond distance labels. At smaller angles the labels, produced from subroutine BOND, are drawn without perspective to prevent excessive foreshortening.
	FS(3,3,48)	Rotation matrices for input symmetry operations based on triclinic system. Used with TS array.
P	IN	Logical number for monitor input magnetic tape.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling ("Tilted Titles").
	KD(5,10)	Part of vector search code array. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
P	LTNO	Logical tape number for magnetic plotting tape.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction (vector search codes).

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

P	NG	FAULT INDICATOR (see 3.4).										
	NJ	Instruction number/100.										
	NJ2	Last two decimal digits of the instruction number (instruction - NJ*100 - NJ2).										
P	NOUT	Logical number for monitor output magnetic tape.										
P	NSR	Logical number for scratch magnetic tape.										
	NSYM	Number of input symmetry operations.										
P	ORGN(3)	Triclinic coordinates for the atom which is the origin of the drawing (i.e., on the optic axis for the projection).										
	P(3,100)	Triclinic positional coordinates for the input atoms.										
	PA(3,3,100)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 Å long, based on the triclinic system (principal axis vectors).										
	PAC(3,5)	A 3 × 3 matrix produced by subroutine PAXES and made up of three orthonormal principal axis column vectors, based on either the working or reference Cartesian system. Columns 4 and 5 are used in subroutine F700 to duplicate columns 1 and 2 for ease in indexing.										
	PAT(3,3)	A matrix produced by subroutine PAXES and composed of three principal axis column vectors each 1 Å long, based on the triclinic system.										
	Q(3,3)	A matrix produced by subroutine PAXES. Contains either the dispersion matrix or its inverse, based on either the working or reference Cartesian systems.										
	REFV(3,3)	A matrix made up of three orthogonal column vectors, each 1 Å long, based on the triclinic system. This is the base vector triplet for the reference Cartesian coordinate system. The transpose is the postfactor transformation matrix for converting coordinates from the reference orthogonal system to the triclinic system. $REFV^T = AAREV^{-1}$.										
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. <table><tr><td>$x = Res(1)$</td><td>128-point ellipse</td></tr><tr><td>$Res(1) \cdot x = Res(2)$</td><td>64-point ellipse</td></tr><tr><td>$Res(2) \cdot x = Res(3)$</td><td>32-point ellipse</td></tr><tr><td>$Res(3) \cdot x$</td><td>16-point ellipse</td></tr><tr><td>$Res(4)$ is not used.</td><td></td></tr></table>	$x = Res(1)$	128-point ellipse	$Res(1) \cdot x = Res(2)$	64-point ellipse	$Res(2) \cdot x = Res(3)$	32-point ellipse	$Res(3) \cdot x$	16-point ellipse	$Res(4)$ is not used.	
$x = Res(1)$	128-point ellipse											
$Res(1) \cdot x = Res(2)$	64-point ellipse											
$Res(2) \cdot x = Res(3)$	32-point ellipse											
$Res(3) \cdot x$	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. $WRKV^T = AAWRK^{-1}$.
P	XLNG(3)	Elements (1) and (2) are x and y plot dimensions. Element (3) is not used.
P	XO(3)	Elements (1) and (2) denote the position in plotter coordinates (in inches) where ORGN is placed. Element (3) is used to transfer Z coordinates to subroutine DRAW when perspective lettering is used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.

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

5. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS

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

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

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

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

If the integration is carried over all space, then

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.2 Equiprobability Ellipsoids

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

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

where

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

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

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

$$P(C) = (2/\pi)^{3/2} \int_0^C r^2 e^{-r^2/2} dr. \quad (5.2.3)$$

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

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

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

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

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

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

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

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

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

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

Table 5.1. Critical values for probability ellipsoids of a trivariate normal distribution^a

P	C	P	C	P	C
0.01	0.3389	0.41	1.3842	0.81	2.1824
0.02	0.4299	0.42	1.4013	0.82	2.2114
0.03	0.4951	0.43	1.4183	0.83	2.2416
0.04	0.5479	0.44	1.4354	0.84	2.2730
0.05	0.5932	0.45	1.4524	0.85	2.3059
0.06	0.6334	0.46	1.4695	0.86	2.3404
0.07	0.6699	0.47	1.4866	0.87	2.3767
0.08	0.7035	0.48	1.5037	0.88	2.4153
0.09	0.7349	0.49	1.5209	0.89	2.4563
0.10	0.7644	0.50	1.5382	0.90	2.5003
0.11	0.7924	0.51	1.5555	0.91	2.5478
0.12	0.8192	0.52	1.5729	0.92	2.5997
0.13	0.8447	0.53	1.5902	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	5.5316
0.40	1.3672	0.80	2.1544	0.9999999	5.9501

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

where

$\mathbf{h}$ is a vector giving the Miller indices,

$\mathbf{X}_n$ is a vector giving the fractional unit cell coordinates of the n th atom,

$\mathbf{B}_n$ is the anisotropic temperature factor coefficient matrix, and

$f_n(\mathbf{h})$ is the atom form factor value for atom n .

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

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

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

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

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

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

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

which is identical to (5.1.3).

5.4 Principal Axis Transformation

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

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

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

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

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

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

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

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

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

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

premultiplying by M yields

$$\left[MG^{-1} - \frac{1}{\lambda_i} I \right] y_i = 0 \quad (i = 1, 2, 3). \quad (5.4.4)$$

Or we can do some additional rearranging and obtain

$$[GM^{-1} - \lambda_i I] y_i = 0 \quad (i = 1, 2, 3). \quad (5.4.5)$$

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

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.

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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.

6.2 Stereoscopic Drawings of Crystal Structures

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

6.2.2.4 Abnormal Motion in Cr(III) Acetylacetonate. — Dr. Bruno Morosin from Sandia Corporation sent this most unusual example of thermal motion. Cr(III) acetylacetonate¹⁵ 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 Chloronateate. — A molecule of this structure¹⁶ is shown in Fig. 6.10. Packing diagrams were also drawn by Ellison and Levy and are reproduced here. Figure 6.17 shows the packing of anions about the two types of potassium ions. One coordination polyhedron is an irregular octahedron of oxygen atoms. The other is an irregular 14-hedron having six oxygen atoms and four chlorine atoms at its vertices. Figure 6.18 is a different view of the packing with a larger area included.

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

An approach which is fairly successful is the following:

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

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

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

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

¹⁵B. Morosin, *Acta Cryst.* 19, 131 (1965) and B. Morosin, private communication, 1964.

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

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

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

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

6.3 Helical Structures

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

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

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

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

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

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

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

6.1 Nonstereoscopic Drawings Showing Thermal Motion

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Fig. 6.11. A Molecule of Ethylenediamine with Thermal Ellipsoids Scaled to Enclose 40% Probability.

BETA-TRICAPSIN
22/6/84 D

BETA-TRICAPSIN
22/6/84 C

Fig. 6.12. Two Molecules of Beta-Tricapsin 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-butanone-1-ene)-Cu(II) with Thermal Ellipsoids Scaled to Include 50% Probability.

Fig. 6.14. A Molecule of the Plant Pigment Muringenin with Thermal Ellipsoids Scaled to Include 40% Probability.

Fig. 6.15. A Unit of *Tris-acetylacetonatechromium(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-acetylacetonatechromium(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. Picking Diagram for Potassium Permanganate 9-Hydrate, Illustrating the Network of Highly Hydrated Potassium Ions Surrounding Permanganate 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 (2-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. Stereoviewing is accomplished by placing a sheet of cardboard between the helices.

7. FORTRAN LISTING OF OR TEP-II

TOTAL NUMBER OF CARDS INCLUDING DATA FOR EXAMPLE IS 874	MAIN	10
ONE STAGE SERIAL ALGORITHM PLOT PROGRAM *****	MAIN	20
*****	MAIN	30
OPTIONAL OVERLAP PHOTOS ADDED TO OVERPLOT IN FEBRUARY 1971 *****	MAIN	40
CURRENT STAMPEL CARDS ILLUSTRATE USE OF OVERLAP PHOTOS *****	MAIN	50
IN OVERPLOT, INSTRUCTIONS 411 MAY BE USED JUST BEFORE EACH	MAIN	60
*****	MAIN	70
WITH INSTRUCTIONS 411 CANNOT PROJECTED BORDERS ALSO TO BE STORED	MAIN	80
*****	MAIN	90
*****	MAIN	100
*****	MAIN	110
*****	MAIN	120
*****	MAIN	130
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P900	150
P901	160
P902	170
P903	180
P904	190
P905	200
P906	210
P907	220
P908	230
P909	240
P910	250
P911	260
P912	270
P913	280
P914	290
P915	300
P916	310
P917	320
P918	330
P919	340
P920	350
P921	360
P922	370
P923	380
P924	390
P925	400
P926	410
P927	420
P928	430
P929	440
P930	450
P931	460
P932	470
P933	480
P934	490
P935	500
P936	510
P937	520
P938	530
P939	540
P940	550
P941	560
P942	570
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P944	590
P945	600
P946	610
P947	620
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P949	640
P950	650
P951	660
P952	670
P953	680
P954	690
P955	700
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P959	740
P960	750
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P962	770
P963	780
P964	790
P965	800
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P967	820
P968	830
P969	840
P970	850
P971	860
P972	870
P973	880
P974	890
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P977	920
P978	930
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P980	950
P981	960
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P983	980
P984	990
P985	1000

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225 0L32,H,1)=72L(J,2),J)      LAPS 142
C 230 EVALUATE COORDINATE POINTS AT NEW POINT Y4 ***** LAPS 143
      Y4(1)=Y(1)                LAPS 144
      Y4(2)=Y(2)                LAPS 145
      Y4(3)=1.0                 LAPS 146
      NPH=NPYH                   LAPS 147
      IF(NCQYTH) 340,350,335    LAPS 148
235 DO 304 K=1,NCQYTH           LAPS 149
      X(1)=YH(1)*CQYTH(1,K)+YH(2)*CQYTH(2,K)+CQYTH(3,K) LAPS 150
      X(2)=YH(1)*CQYTH(2,K)+YH(2)*CQYTH(3,K)+CQYTH(4,K) LAPS 151
      X(3)=YH(1)*CQYTH(3,K)+YH(2)*CQYTH(4,K)+CQYTH(5,K) LAPS 152
      CQIH,2)=X(1)*YH(1)+X(2)*YH(2)+X(3) LAPS 153
C 0000 EVALUATE COORDINATE POINTS FOR NEW IS DONE ***** LAPS 154
      IF(NPH=1) 308,307,305    LAPS 155
240 CQIH=X(1)*YH(1)+X(2)*YH(2)+X(3) LAPS 156
245 CONTINUE                    LAPS 157
C 0000 EVALUATE LINEAR POINTS AND SIGNATURE FOR QUADRANGLE ***** LAPS 158
250 IF(NH=0) 275,275,255       LAPS 159
255 DO 250 K=1,NH              LAPS 160
      J2=J,0                   LAPS 161
      DO 264 J=1,6             LAPS 162
      Y1=YH(1)*CQYTH(1,J)+YH(2)*CQYTH(2,J)+CQYTH(3,J) LAPS 163
      IF(Y1) 260,264,264       LAPS 164
      J2=J2-1.0               LAPS 165
264 0L(J,H,2)=Y1               LAPS 166
      H2=H2+1                  LAPS 167
C 0000 J2=-1 INSIDE, +1 ACROSS ANY EDGE, =1 ACROSS ANY VERTEX ***** LAPS 168
270 CQIH(2,J)=J2               LAPS 169
C 0000 IF PTH IS UP, ONLY ALL SUBSEQUENT CHECKING ***** LAPS 170
275 IF(NH=1) 294,293,290       LAPS 171
280 NPH=1                       LAPS 172
      CALL XCP1P(YH,NPH,LTHC)   LAPS 173
      RETURN                    LAPS 174
C 0000 CHECK FOR HIDDEN SEGMENT ***** LAPS 175
285 DO 294 K=1,NCQ            LAPS 176
      IF(CQIH,1) 300,304,304    LAPS 177
290 IF(CQIH,2) 300,304,305     LAPS 178
295 CONTINUE                   LAPS 179
C 0000 FIND ENTRY AND EXIT POINTS ON EACH COORD ***** LAPS 180
      NINT=0                    LAPS 181
      IF(NCQYTH) 310,310,300    LAPS 182
300 DO 325 K=1,NCQYTH          LAPS 183
      0000 EVALUATE DISCRIMINANT ***** LAPS 184
      Y1=CQIH(1)*CQIH(1,K)+CQIH(2) LAPS 185
      IF(Y1) 325,325,305       LAPS 186
305 Y1=SQRT(Y1)                LAPS 187
      0000 SOLVE QUADRATIC EQUATION ***** LAPS 188
      J2=CQIH,1)-CQIH(1)        LAPS 189
      Y1=Y2+CQIH,2)-CQIH(2)     LAPS 190
      IF(ABS(Y1)-1.0) 325,325,310 LAPS 191
310 Y4=(Y2-Y1)/Y1              LAPS 192
      Y5=(Y2+Y1)/Y1             LAPS 193
C 0000 VALID INTERSECTION IF Y4,LT,1 AND Y5,GT,0 ***** LAPS 194
      IF(YH-1.0) 315,325,325    LAPS 195
      IF(Y5) 325,325,320        LAPS 196
C 0000 HAVE VALID COORD INTERSECTIONS ***** LAPS 197
320 RETURN                     LAPS 198
      SIGN(INTR,1)=YH           LAPS 199
      SIGN(OUT,2)=Y5            LAPS 200
325 CONTINUE                   LAPS 201
330 IF(NH=0) 325,325,335       LAPS 202
C 0000 FIND ENTRY AND EXIT POINTS FOR EACH QUADRANGLE ***** LAPS 203
335 DO 340 K=1,NH              LAPS 204
      I12=0                     LAPS 205
      H2=H2+1                   LAPS 206
C 0000 CHECK FOR SINGLE INSIDE POINT ***** LAPS 207
      XH(1)=CQIH(2,1)           LAPS 208
      IF(XH(1)) 340,340,300     LAPS 209
340 IF(XH(1)=1.0) 350,350,305   LAPS 210
      IF(XH(1)-1.0) 350,350,305 LAPS 211
C 0000 INSIDE POINT FOUND, ONLY ONE INTERSECTION POSSIBLE ***** LAPS 212
345 I12=1                       LAPS 213
C 0001 FIND WHICH POINTS ARE CHANGED BY THE SEGMENT ***** LAPS 214
350 DO 410 J=1,6               LAPS 215
      Y1=0L(J,H,1)              LAPS 216
      Y2=0L(J,H,2)              LAPS 217
      J3=Y1-Y2                  LAPS 218
      IF(Y1-Y2) 355,355,410     LAPS 219
C 0000 CHECK FOR SEGMENT ON AN EDGE ***** LAPS 220
355 IF(ABS(Y1)-1.0) 420,420,360 LAPS 221
C 0000 CALCULATE COORDINATES OF INTERSECTION ***** LAPS 222
360 Y4=(Y1*YH(1)+Y2*YH(2))/Y3   LAPS 223
      Y5=(Y1*YH(2)+Y2*YH(3))/Y3 LAPS 224

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242 PA(J,1)=PA(J,1)+.5
    DO 70 J=1,30
    ***** TYPED 3 ADD 1 (BASE 3 SYSTEM) *****
244 TA=.15152000
    IP(J)=200,200,200
    ***** TYPED 4 THROUGH 4 *****
270 IF(PA(J,1)) 000,000,272
272 DO 100 J=1,1
    DO 100 L=J,1
    72=74
    IF(M=-1)204,274,274
274 IF(M=-1)200,200,201
    ***** TYPED 8 ADD 5 *****
280 IF(PA(J)=0)1070,20
    DO 70 J=1,1
    ***** TYPED 8 ADD 9 (01,1) THROUGH SYSTEM) *****
281 T2=0(J)=0(L)
    IF(L=1)204,207,207
    ***** TYPED 10, (CAPTEIAN THROUGH SYSTEM) *****
282 7=1.0
204 IF(J=1)200,207,200
207 VT(J,1)=T2*PA(J,1,1)
    DO 70 J=0
290 H=J+1
    VT(J,1)=T2*PA(H,1,1)
    VT(L,1)=VT(J,L)
300 CONTINUE
    ***** TYPED PRINCIPAL AREA *****
    IF(M=-1)110,104,104
304 CALL QN(VT,0,PAC)
    CALL QN(DTTP,PAC,VT)
310 CALL QN(VT,10,DA)
    CALL TYPED100,0N,PAT)
    ***** ARE THROUGH LINE POSITIVE *****
    IF(0N(1))224,224,270
320 IF(0N)140,140,110
324 0N=1
330 0N=1
    CALL SUBPT(PL0AT(1)=0000,+.5501,0)
    ***** 1 EQUAL THROUGHPUTS, ONE DIFFERENCE THROUGH *****
340 T1=000000007(ABS(0N(1)-0N(2)+0N(3))/3),0N(1))
    DO 100 J=1,1
    DO 100 L=J,1
342 PA(J,0,1)=DTTP(J,0)
344 VT(J,1)=0
    DO 70 040
346 IF(0N(1))100,100,142
    ***** TWO EQUAL THROUGHPUTS *****
348 0N=0.4
    CALL QN1(PAT(1,0),V1,-1)
    DO 140 001,1
    IF(ABS(0NPT(1,0A,0NPT(1,0)))-.001)140,140,140
348 CONTINUE
348 CALL QN(10,0A,0N)
    CALL 02TP(01,0NPT(1,0),0A,-1)
    DO 140 001,1
    L=0N(0N(2,1)+1)
    DO 140 J=1,1
348 PA(J,L,1)=PA(J,0)
348 VT(J,1)=270000007(ABS(VV(PA(1,0),VT,PA(1,0))),0N(1))
    DO 70 040
    ***** ONE THROUGHPUTS 1 AND THROUGH LONG *****
360 CALL 02TP(PAT(1,1),PAT(1,1),PA(1,1),-1)
370 0N=1
    ***** 0000 THROUGHPUT = ONE DIFFERENCE *****
    DO 174 J=1,1
    T2=0N(01)
374 VT(J,1)=100000007(ABS(T2)),T2)
    DO 70 040
    ***** TYPE 4 (THROUGHPUT TEST FACTOR) *****
400 T1=0000007(1,30045E-3)
    ***** TYPE 7 (000000 SPHERE) *****
404 DO 010 J=1,1
410 VT(J,1)=01
    IF(PA(1,1))010,010,014
    ***** 000000000000 TWO SPHERE *****
414 DO 024 J=1,0
    T2=0N(J),1,1)
    CALL 0700(T2,VT(1,1))
    IF(0N)020,024,020
420 CALL 0000(T2,1)
    DO 70 010
424 CONTINUE
    CALL 01TP(VT(1,1),VT(1,1),VT(1,1),VT(1,1))

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PDEL 1760
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