3. ORTEP INPUT

3.1 DEFINITIONS

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

3.1.1 Atom Designator Code (ADC) and Addressable Point

A five-component *atom designator code* is used to specify a particular atom in the crystal within a reasonable distance from the crystallographically defined origin.

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

where

AN = *atom number (*$0 \leq \text{AN} \leq \text{NATOM} \leq 500$) – the numerical position of the atom in the input list of atoms in the asymmetric unit, which contains NATOM atoms. Atom 0 is not in the input atom list but refers to the crystal origin point (0.,0.,0.).

TA,TB,TC = *crystal lattice translation digits* – translations along cell edges **a**, **b**, and **c**, respectively. Each digit in an ADC can range from 1 to 9; consequently, it is possible to move up to 4 cells in any direction from the origin cell 555.

SN = *symmetry operator number (*$0 \leq \text{SN} \leq \text{NSYM} \leq 96$) – the numerical position of the symmetry operator in the input list of symmetry operators, which contains NSYM entries. Symmetry operator number 0 is not in the input list but refers to an identity operator. However, the identity operation (corresponding to position *x, y, z*) generally must be somewhere in the input symmetry operator list and is usually the first operator.

Example: An atom designator 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 designator code* defines a vector using 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)

An *atom designator run* is a straight run sequence of atoms that is defined using two atom designator codes with a “-” preceding the second of the two. The run hierarchy is: first, atom number AN; second, symmetry operator number 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.

The following exceptions are allowed in Org. ADRs of instructions 101, 102, 402/412, 403/413, and 404/414 **only**:

- The "-" may be omitted from the second ADC.
- If the second atom in the atom designator run has the same symmetry and translation components as the first atom, the second atom may be represented by its atom number component alone.
- If the symmetry and translation components of both atoms are 55501, both atoms may be represented by their atom number components alone.

Example: ADR (345502-745502) may also be represented as (345502 745502) or (345502 7). ADR (355501-755501) may also be represented as (355501 755501) or (355501 7) or (3 7).

3.1.4 Atom Number Run (ANR)

An *atom number run* is a subset of the atom designator run in which only the atom number AN changes. Normally, an ANR is entered by using only the atom number values for the first and last members of the sequence without a "-".

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 number runs and a distance range. It is used for finding interatomic distances that 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, oxygen atoms are 6-12, and 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 ORTEP.

The vector searches in ORTEP-III for the 100 instructions and 400 instructions have been generalized to allow both atom number runs and feature number runs (see 3.1.11) with the number run type (see 3.1.12) specified in column 24. In addition, it is no longer necessary to specify all three screening ranges found on this card (i.e., origin, target, and distance range). Any ranges not specified (i.e., zero or blank in the maximum value entry) are omitted from the screening. If there is more than one vector search card for an instruction, the parameter LOGC controls the logic of the screening. If the value is "0" (the default), an atom satisfying the screening conditions on any one of the No. 2 trailer cards will be retained (i.e., it is a logical union of the results). If the value is "1", an atom must satisfy the screening conditions on all the cards to be retained (i.e., it is an intersection of the results). If a value of "1" is needed for LOGC, a "1" is placed in column 27 of a Format No. 1 trailer card that goes between the main instruction card and the Format No. 2 VSC cards. If the value for LOGC is "0", the Format No. 1 card is not needed.

3.1.6 Sphere of Enclosure

A *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. The 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 that are derived from a group of sequential atoms in the input list or atoms having particular features, 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 (see 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 the origin atom should not be chosen in the outermost cells because of the possibility of having nonaddressable points within the D_{max} radius.

3.1.7 Box of Enclosure

A *box of enclosure* is a parallelepiped that can be centered about any addressable point and assigned arbitrary orientation and dimensions. The orientation depends upon either the unit cell axes (triclinic box of enclosure) or the reference axes (rectangular box of enclosure). The box of enclosure can have a *complete population,* a *partial population,* or a *vector screened population* as described for the sphere of enclosure (see 3.1.6).

3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems

Many of the ORTEP calculations use fractional coordinates based on the crystal axes $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ (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 series 500 instructions. Until a 500-series instruction is given, a "standard Cartesian system" is utilized for both the reference and working systems. The orthonormal base vectors of the standard system are oriented as follows:

$$x \text{ axis along } \mathbf{a},$$

$$y \text{ axis along } (\mathbf{a} \times \mathbf{b}) \times \mathbf{a},$$

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

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

3.1.9 Prime Parameters and Primer Constants

The more basic among the many settable parameters in ORTEP are the *prime parameters.* The default values assigned to these prime parameters are often similar or identical from one problem to the next. Among the first things ORTEP does is a call to subroutine PRIME, which sets as many prime parameters as possible to reasonable default *primer constant* values. For example, the maximum plot dimensions (instruction 301) are set to 10.5 in. for x_{max} and 8.0 in. for y_{max}, and the overall scale for plotting (instruction 600 series) is set to 1.0 in./Å. If the value assigned to a particular constant by the PRIME subroutine is satisfactory, the user does not have to change the value with ORTEP instructions.

3.1.10 Atom Feature

An *atom feature* is a user-defined characteristic of a group of atoms that may be assigned to the atoms in the ORTEP input as needed for a given task. For example, the atomic number may be provided with each atom to make selecting atoms of the same element easier. Up to two features may be assigned to each atom. These are referred to as Feature #1 and Feature #2. (See 4.6.)

3.1.11 Feature Number Run (FNR)

A *feature number run* is used to identify those atoms having a particular atom feature within a specified value range.

3.1.12 Number Run (NR) and Number Run Type

A *number run* is a generic term that refers to both atom number runs (ANR) (see 3.1.4) and feature number runs (FNR) (see 3.1.11). The *number run type* identifies the number run. Number run type 0 refers to an ANR, type 1 refers to an FNR on Feature #1, and type 2 refers to an FNR on Feature #2.

3.2 CRYSTAL STRUCTURE DATA INPUT

3.2.1 Title

The first card in the ORTEP input is a title card with FORMAT (18A4), consisting of up to 72 characters of alphanumeric identification information. This will appear periodically in the output file.

3.2.2 Cell Parameters

The second input card contains the cell parameters with FORMAT (I1,F8.6,5F9.6). Any one of the following four input alternatives may be used.

Columns	Type A	Type B	Type C	Type D
1	Symmetry format indicator	Symmetry format indicator	Symmetry format indicator	Symmetry format indicator
2-9	**a** (Å)	**a** (Å)	**a*** (Å^{-1})	**a*** (Å^{-1})
10-18	**b** (Å)	**b** (Å)	**b*** (Å^{-1})	**b*** (Å^{-1})
19-27	**c** (Å)	**c** (Å)	**c*** (Å^{-1})	**c*** (Å^{-1})
28-36	α (°)	cos α	α^* (°)	cos α^*
37-45	β (°)	cos β	β^* (°)	cos β^*
46-54	γ (°)	cos γ	γ^* (°)	cos γ^*

No indicator is needed to specify the input type. The routine assumes that $\mathbf{a} \geq 1.0$ Å, $\mathbf{a}^* < 1.0$ Å^{-1}, α (or α^*) $\geq 1.0°$, and $|\cos\ \alpha|$ (or $|\cos\ \alpha^*|$) < 1.0. The parameters $\mathbf{a}^*$, etc., refer to the reciprocal unit cell such that $\mathbf{a}\cdot\mathbf{a}^* = 1$. All four types will be printed in the output regardless of which type was used for input.

An integer value in column 1 of the cell parameter card indicates the format used for the crystal symmetry cards that follow.

3.2.3 Symmetry

Crystal symmetry in ORTEP-III may be supplied in either of two styles. The first of these is identical to that of OR TEP-II[2] and is triggered by having a "0" or blank in column 1 of the cell parameter card. A "1" in that position indicates the symmetry operators are provided in a free format using the xyz coordinate triplet notation found in the International Tables for Crystallography.[4] These two styles are referred to as Type 0 and Type 1, respectively.

The number of symmetry cards (NSYM) may not exceed 96. At least one (the identity operator) is required. The reason for the maximum of 96 is that the *symmetry operator number* (SN) occupies only two places in the ADC (see Sect. 3.1.1). If it is not possible to supply all the symmetry operators for the space group (or if the user chooses not to supply all of them), each unique atom in the ORTEP input file will require multiple entries with those lattice centering translations added that are not provided in the symmetry cards. (See 7.5 for an example.)

A Type 0 symmetry card has FORMAT (I1,F14.10,3F3.0,2(F15.10,3F3.0)) and will be interpreted in one of two ways, depending on the value of the number in columns 70-72. If that number is < 5.0, the card is interpreted as a crystallographic symmetry operation; but if the number is ≥ 5.0, the card is interpreted as a general helix-screw symmetry operation[†] along the $\mathbf{c}^*$ crystal axis (third axis of the standard Cartesian system; see 3.1.8). The two symmetry types can be intermixed if desired.

---

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

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

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

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

or in matrix notation

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

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

Only symmetry cards for *general* symmetry equivalent positions are permitted. Symmetry cards that explicitly designate special positions such as X,X,X; X,X,Z; $X,Y,0$; $1/4,Y,0$; and 1/4,3/4,0 are *not allowed*.

(b) Helix screw symmetry:

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

where $\mathbf{T} = (T_1,T_2,T_3+L/N)$ as fractions of cell edges and $\mathbf{S}$ is a counterclockwise rotation of $L{\cdot}M/N$ cycles about the $\mathbf{c}^*$ axis.

Example: The Pauling and Corey right-handed alpha helix of poly-L-alanine repeats after 13 turns and 47 residues and can be represented by 47 symmetry cards with $N = 47$; $M = 13$; $L = 0, 1, \ldots, 46$; $T_1, T_2, T_3 = 0$. The input atom list then contains the contents of one residue. (See 7.2.)

Type 1 crystallographic symmetry cards do not have a specific format with the following two exceptions: (1) the symmetry information on each card must not go beyond column 72, and (2) column 1 must be "0" (or blank) on all symmetry cards other than the last one in the set, which must be non-zero. Below is an example set of Type 1 symmetry cards to illustrate the flexibility of this style.

```
 X,Y,Z
 X    -Y   Z+1/2
   X+0.5,   Y+.5,  Z
1x+1/2,-y+1/2,1/2+z
```

As shown, letters may be either upper or lower case. Commas or blanks may be used to separate the components of the triplet. The three components may not have blanks within them. Decimal fractions may be used with or without an initial 0. Fractions may precede or follow the letters.

Regardless of how the symmetry information is provided, the last card of the set must have a non-zero value in column 1 to signal the end of the symmetry cards. If the value is "1", the atom parameter information immediately follows in the ORTEP input file as described in Section 3.2.4. If the value is "2", the atom parameter information is read from a different file (see 4.5), and the ORTEP instructions follow the symmetry cards.

3.2.4 Atom Parameters

Two cards are required for each input atom. The first contains the chemical symbol , positional parameters, and feature information, if needed, The second contains temperature factor information or other information that specifies how the atom is to be represented on the drawing. Several alternate inputs are possible for each of the two cards, and the number in column 63 denotes the type used on that particular card. The number of atoms (variable NATOM) may range from 1 to 500.

3.2.4.1 Positional Parameters

The positional parameter cards have FORMAT (A6,3X,6F9.0).

Columns	Type 0	Type 1	Type 2	Type 3
1-6	Up to six alphanumeric characters centered in the six-place field			
7-9	—			
10-18	[Feature #1]	[Feature #1]	[Feature #1]	x_0 (Å, Cartesian)
19-27	[Feature #2]	[Feature #2]	[Feature #2]	y_0 (Å, Cartesian)
28-36	x (fractional, crystal)	x (Å, crystal)	x (Å, Cartesian)	r (Å, cylindrical)
37-45	y (fractional, crystal)	y (Å, crystal)	y (Å, Cartesian)	ϕ (°, cylindrical)
46-54	z (fractional, crystal)	z (Å, crystal)	z (Å, Cartesian)	z (Å, cylindrical)
63	0	1	2	3

Type 0 is the normal input based on triclinic coordinates. Coordinates in Angstroms along the unit cell vectors may be entered with Type 1. Type 2 may be used to place a model described in Cartesian coordinates onto a general triclinic lattice. The orientation of the Cartesian system *xyz* in the general lattice **abc** is the standard type described in Section 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 *xy* Cartesian plane by the displacement x_0, y_0. Cylindrical coordinates are often used to describe helical structures. The x_0, y_0 translation should be zero if helical symmetry operators are used. This translation feature is meant to be used for explicitly describing the contents of a multiple helix cell.

Column fields 10-18 and 19-27 on Type 0, 1, and 2 positional parameter cards may be used in ORTEP-III to enter "feature" information about the atoms (see 3.1.10 and 4.6). Normally, these fields are ignored by ORTEP so any numeric values may be here or the fields may be blank. The information in these fields will be interpreted as atom features only if instructions are invoked that specifically look at atom features. Features cannot be entered on Type 3 positional parameter cards.

3.2.4.2 Temperature Factors

Temperature factor cards have FORMAT (I1,F8.0,5F9.0,7X,F2.0).

Columns	Type 0,1,2,3,10	Type 4,5,8,9	Type 6		Type 7	
1	A sentinel ≠ 0 for last atom only					
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 (from)	0	VDC_1 (from)
28-36	b_{12}	U_{12}	0	VDC_1 (to)	0	VDC_1 (to)
37-45	b_{13}	U_{13}	0	[VDC_2 (from)	0	[VDC_2 (from)
46-54	b_{23}	U_{23}	0	VDC_2 (to)]	0	VDC_2 (to)]
55-63	0,1,2,3,10	4,5,8,9	6 (or 0)	6 (or 0)	7	7

Anisotropic temperature factor Types 0, 1, 2, 3, and 10 use the following formula for the complete temperature factor.

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

The coefficients $b_{ij}(i,j = 1,2,3)$ of the various types are defined with the following constant settings.

Type 0:	Base = e, $c = 2$, $D = 1$
Type 1:	Base = e, $c = 1$, $D = 1$
Type 2:	Base = 2, $c = 2$, $D = 1$
Type 3:	Base = 2, $c = 1$, $D = 1$
Type 10:	Base = e, $c = 2$, $D = 2\pi^2$

Anisotropic temperature factor Types 4, 5, 8, and 9 use the following formula for the complete temperature factor, in which $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ are reciprocal cell dimensions.

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

The coefficients $U_{ij}\,(i,j = 1,2,3)$ of the various types are defined with the following constant settings.

Type 4:	$C = 2,\ D = \frac{1}{4}$
Type 5:	$C = 1,\ D = \frac{1}{4}$
Type 8:	$C = 2,\ D = 2\pi^2$
Type 9:	$C = 1,\ D = 2\pi^2$

Type 6 allows the input of the Debye-Waller isotropic temperature factor $B,$ which is used as follows:

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

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

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

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

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

If VDC_2 is omitted on Type 6 or Type 7 temperature factor cards, the program will choose one of the three lattice vectors for VDC_2.

A Type 10 temperature factor input card may be used to load Cartesian temperature factors having components in the standard Cartesian system (see 3.1.8). This capability complements the Type 3 Cartesian positional parameter input system (see 3.2.4.1) and is useful for plotting mean-square displacements caused by internal molecular motions as calculated from spectroscopic normal-coordinate analyses.[6,7]

New in ORTEP-III is the method for specifying the orientations and sizes of the elongated pass (cigar-shaped) and flattened pale (pancake-shaped) ellipsoids used in critical net illustrations (see 7.5) without giving their quadratic form coefficients. The temperature factor card following the atom parameter card for a pass or pale has the format shown below.

Columns	
1	A sentinel ≠ 0 for last atom only
2-9	Unique axis length (Å)
10-18	Second (and third) axis length (Å)
19-27	VDC_1 (from)
28-36	VDC_1 (to)
37-45	[VDC_2 (from)
46-54	VDC_2 (to)]
63	7

VDC_1 is a vector parallel with the unique axis of the cigar-shaped pass or pancake-shaped pale and VDC_2 is a second vector **not** parallel with VDC_1 such that $VDC_1 \times VDC_2$ is a second principal axis of that ellipsoid. If VDC_1 and VDC_2 are parallel, VDC_2 is replaced by a suitable lattice translation vector. VDC_2 may be omitted from the input if desired, and the program will choose one of the three lattice vectors for VDC_2.

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.

3.3.1 Instruction Format

There are four different formats used for ORTEP instructions, which are numbered 0, 1, 2, and 3. Format No. 0 is always used for a new instruction and includes the instruction number. Some instructions require trailer (continuation) cards, which use Format Nos. 1, 2, and 3. The program is informed what the format of the next card will be with the value in the “look ahead” field, column 3. The program action is also influenced by this information.

“Look ahead” on current card (column 3)	Next card will be	Program action
0 or blank	Format No. 0, a new instruction	Execute present instruction; then read next new instruction card
1	Format No. 1, continuation of present instruction	Read continuation card and then check its “Look ahead”
2	Format No. 2, continuation of present instruction	Read continuation card and then check its “Look ahead”
3	Format No. 3, alphanumeric information	Read alphanumeric information and execute instruction; then read next new instruction card

The Format No. 0 instruction card and the Format No. 1 parameter continuation card have the FORMAT (I3,I6,7F9.0), but the former includes the instruction number while the latter does not. A maximum of 19 Format No. 1 continuation cards per instruction is permitted.

Columns	**Format No. 0 Instruction Card**	**Format No. 1 Parameter Continuation Card**
3	"Look ahead" (0,1,2,3)	"Look ahead" (0,1,2,3)
4-9	Instruction number	Blank
10-18	1st parameter	8th parameter, or 15th, …, or 134th
19-27	2nd parameter	9th parameter, or 16th, …, or 135th
…	…	…
64-72	7th parameter	14th parameter, or 21st, …, or 140th

The Format No. 2 trailer card is also used for parameter continuation, but it is more compact with FORMAT (I3,6X,5I3,8F6.0), allowing more information to be entered than on the Format No. 1 card. Many, but not all, Format No. 2 trailer cards include vector search codes (see 3.1.5), and they are often referred to as Vector Search Code (VSC) cards. A maximum of 20 Format No. 2 continuation cards per instruction is permitted.

Columns	**Format No. 2 Parameter Continuation Card**
3	"Look ahead" (0,1,2,3)
4-9	—
10-12	1st integer parameter
…	…
22-24	5th integer parameter
25-30	1st real parameter
…	…
67-72	8th real parameter

Format No. 3 trailer cards with FORMAT (18A4) are used for entering label information and are required for instructions 902, 903, and 913. As a trailer to these, they may contain up 72 characters of alphanumeric information in columns 1-72, centered about columns 36 and 37 or beginning in column 1 for automatic centering. These may also be used with other instructions as a device to transfer comments about the particular instruction to the ORTEP output listing. There is no "look ahead" column in Format No. 3; the next card must be a new instruction card.

3.3.2 Structure Analysis Instructions (100 Series)

This series of instructions is not connected with drawing illustrations but rather with obtaining a convenient tabulation of the chemically interesting aspects of a crystal structure, including interatomic distances and angles and principal axes of thermal motion. If the ORTEP output is omitted (see 4.1), these instructions do nothing.

3.3.2.1 Instructions 101 and 102

These instructions call subroutine SEARC, 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 one or several origin atoms (Org. ADR) and an atom number run of target atoms (Tar. ANR). The Org. ADR allows calculation of several spheres successively with a printout of results after each one.

Example: Suppose there are nine atoms in the input list and we want to find all atoms surrounding atoms 365502, 465502, and 565502 out to a maximum radius of 4 Å.

```
        101   365502        5        1        9      4.0
```

The selection of the interatomic vectors from a particular origin atom to the target atoms can be narrowed with a vector search code on a Format No. 2 continuation card (see 3.3.1). The first line of the instruction defines a limiting sphere of vectors, and the VSC finds the subset of vectors that satisfy the additional restriction. (See 3.1.5.)

Example: Suppose we want to limit the results of the search in the preceding example to the shell of atoms that lie 2.0-2.7 Å from each of the origin atoms.

```
    2   101   365502        5        1        9      4.0
               3  5  1  9  0   2.0   2.7
```

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, 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. The tabulation of atom designator codes, which is obtained automatically when these instructions are given, is often useful for planning an illustration.

Columns	Instructions 101 and 102
3	0, 1, or 2
7-9	101 or 102
10-18	Org. ADR (from)
19-27	Org. ADR (to)
28-36	Tar. ANR (from)
37-45	Tar. ANR (to)
46-54	D_{max} (Å)

Columns	Format No. 2 Vector Search Code (if used)
3	0 or 2
4-9	—
10-12	[Org. NR (from)
13-15	Org. NR (to)]
16-18	[Tar. NR (from)
19-21	Tar. NR (to)]
24	[NR type]
25-30	[D_{min} (Å)
31-36	D_{max} (Å)]

Columns	Format No. 1 Continuation Card (if needed)
3	2
7-9	—
10-18	—
27	LOGC

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	Instruction 103
7-9	103
10-72	Blank

3.3.2.3 Instructions 105 and 106, Convoluting Sphere of Enclosure and Reiterative Convoluting Sphere of Enclosure

These instructions utilize the ATOMS array and thus can only be used after one or more atoms have been placed in the table by a $40n$ instruction (see 3.3.5). The contents of the array are returned to the condition of entry at the conclusion of instructions 105 and 106.

All atoms in the ATOMS array that have atom or feature numbers within the origin number run (Org. NR) of the instruction are used as origin points. Interatomic distances for all neighboring atoms (whether or not in the ATOMS array) are found out to the specified radius. Vector search codes on Format No. 2 continuation cards may be used for screening if desired. (See 3.1.5.)

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. NR 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 array with a 401 instruction and let a 106 instruction find the molecule. Care must be taken to specify a D_{max} that will enclose only bonded atoms. The 106 instruction should not be used for structures forming infinite chains. Instead, a short sequence of 105 instructions can be used for this case.

Columns	**Instructions 105 and 106**	Columns	**Format No. 2 Vector Search Code (if used)**
3	0, 1, or 2	3	0 or 2
7-9	105 or 106	4-9	—
10-18	Org. NR (from)	10-12	[Org. NR (from)
19-27	Org. NR (to)	13-15	Org. NR (to)]
28-36	Tar. NR (from)	16-18	[Tar. NR (from)
37-45	Tar. NR (to)	19-21	Tar. NR (to)]
46-54	D_{max} (Å)	24	[NR type]
63	NR type	25-30	[D_{min} (Å)
		31-36	D_{max} (Å)]

Columns	**Format No. 1 Continuation Card (if needed)**
3	2
7-9	—
18	—
27	LOGC

3.3.3 Plotter Control Instructions (200 Series)

The 200 series is a group of instructions that control the device, real or virtual, that receives the information to output the ORTEP illustration. This may be, for example, an actual hardware plotter, a computer monitor, or a file of page description language instructions that will produce a hard copy of the illustration when the file is downloaded to a printer/plotter. Because no single word can describe all of the possibilities, the word "plotter" will be used in this report.

The 200 instructions control plotter initialization, plot origin, color control, 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, the series 200 instructions, which are executed through subroutine F200, should be redefined to suit the user's requirements.

The 201 instruction initializes plotting and must be executed before any plotting can take place. It is a safe policy always to make this the first instruction card. If the 201 and 301 instructions are omitted, all calculations are carried out but no plotting is done. The 202 instruction with no parameters is used to terminate plotting. With parameters, the 202 instruction may be used to shift the plot origin. The 201/202 (with no parameters) form an initialize/terminate pair and must always appear in pairs in the ORTEP input file. The pair *may occur more than once* (unlike OR TEP-II[2]). Each call to 201 begins a new plot page.

Instruction 204 is used to change the color of (or plotter pen used for) subsequent plotting. The default value is 0 for black (or pen #1). The screen and Postscript drivers built into ORTEP-III define color value 2 as red, 3 as green, 4 as blue, 5 as cyan, 6 as magenta, and 7 as yellow. (The value 1 is also black or pen #1.)

Instruction 205 is used to vary the thickness of subsequently plotted lines. The unit for width is thousandths of an inch, and the default value is 5. For both the 204 and 205 instructions, if columns 10-18 contain "0" or are blank, the default settings are restored.

Columns	**Instruction 201**	**Instruction 202**		**Instruction 204**	**Instruction 205**
		Shift plot origin	Terminate plotting		
7-9	201	202	202	204	205
10-18	—	Shift along x (in.)	—	Color (or pen #)	Pen width
19-27	—	Shift along y (in.)	—	—	—

3.3.4 Drawing Parameter Instructions (300 Series)

This is a set of instructions for specifying the drawing dimensions, viewing distance, general lettering orientation, pen displacement for line retracing, and ellipse smoothness.

3.3.4.1 Instruction 301, Drawing Boundaries, Margin, and Viewing Distance

This instruction defines the maximum x and y dimensions of the drawing and the margin, all in inches. 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 drawing margin is a constant width border 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 representation, which has a finite size, may extend into that area. To accommodate this extension into the margin, the margin width 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	**Instruction 301**	Primer Constant
7-9	301	—
10-18	Drawing x_{max} (in.)	10.5
19-27	Drawing y_{max} (in.)	8.0
28-36	View distance (in.)	0. (parallel projection)
37-45	Margin width (in.)	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 the finished drawing has either the y plotter axis vertical or the x plotter axis vertical.

Columns	**Instruction 302**	Primer Constant
7-9	302	—
10-18	θ (°)	0.

3.3.4.3 Instruction 303, Retrace Displacement

Instruction 303 directs certain lines to be made heavier than others by retracing over the path several times with slight pen displacements (DISP) from the original path. For example, if DISP is greater than 0., the forward half of the principal plane trace of ellipsoids is drawn heavier than the hidden half so the eye does not confuse the two halves. Also, all regular lettering (but not perspective lettering) is gone over four times to give it a boldface appearance. In ORTEP-III, retracing is turned off by default with the primer constant for DISP set to 0. in. Retracing can be turned on with the 303 instruction, using a value for DISP greater than 0. (0.005 in. usually works well).

Columns	**Instruction 303**	Primer Constant
7-9	303	—
10-18	DISP (in.)	0.

3.3.4.4 Instruction 304, Ellipse Smoothness

Instruction 304 may be used to adjust the smoothness of the plotted ellipses as a function of their size. Smoother ellipses require more computational time and produce larger illustration files. (See 5.2.) Smaller smoothness factors produce smoother ellipses, and larger values produce ellipses with more “jaggies”. Factors in the range 0.5–3.0 are recommended; the default value is 1. A value of 0 will draw all size ellipses with 128 points, the maximum provided in ORTEP.

Columns	**Instruction 304**
7-9	304
10-18	Smoothness factor

3.3.5 ATOMS Array 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 as currently dimensioned holds 500 input atoms, but it can be changed by redimensioning the array in COMMON and setting the variable NATOM in subroutine PRIME to the new value.

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 40*n* and 41*n* 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 array is printed in the ORTEP output file after each 400 series instruction.

3.3.5.1 Instructions 401/411, Atom Designator Run Add/Eliminate

These instructions may contain: *(a)* atom designator codes for single atoms; (*b*) atom designator runs 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 array and overlap calculation, however, will only accept the first 500 atoms.

Columns	**Instructions 401/411**
3	0 (or 1 if continued)
7-9	401 or 411
10-18	
.	
.	As described above
.	
64-72	

3.3.5.2 Instructions 402/412, Sphere of Enclosure Add/Eliminate

These instructions allow the user to build or modify the ATOMS array by specifying the contents (complete, partial, or vector screened) of a sphere of enclosure (see 3.1.6) about any addressable point. Instruction 402 adds the contents of the spheres to the ATOMS array omitting positional duplications. The 412 instruction eliminates atoms within the spheres from the ATOMS array if they are present in that array. The instructions call subroutine SEARC, 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 ORTEP output file, only the ATOMS array 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 those atom numbers. Vector search codes on Format No. 2 continuation cards may be used for screening if desired. (See 3.1.5.)

Columns	**Instructions 402/412**
3	0, 1, or 2
7-9	402 or 412
10-18	Org. ADR (from)
19-27	Org. ADR (to)
28-36	Tar. ANR (from)
37-45	Tar. ANR (to)
46-54	D_{max} (Å)

Columns	**Format No. 2 Vector Search Code (if used)**
3	0 or 2
4-9	—
10-12	[Org. NR (from)
13-15	Org. NR (to)]
16-18	[Tar. NR (from)
19-21	Tar. NR (to)]
24	[NR type]
25-30	[D_{min} (Å)
31-36	D_{max} (Å)]

Columns	**Format No. 1 Continuation Card (if needed)**
3	2
7-9	—
10-18	—
27	LOGC

3.3.5.3 Instructions 403/413 and 404/414, Box of Enclosure Add/Eliminate and Triclinic Box of Enclosure Add/Eliminate

The 403/413 instructions allow the user to build or modify the ATOMS array by specifying the contents of a box of enclosure (see 3.1.7) about any addressable point (or atom designator run of addressable points). The three axes of the box are parallel to the three base vectors of the reference Cartesian system, and the semidimensions of the box are specified on the instruction card. If an orientation of the box different from the standard orientation (see 3.1.8) is desired, 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.

The 404/414 instructions are identical to the 403/413 instructions 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 (.5,.5,.5).

As in the case of the 402/412 instruction, the origin atom on which the box is centered will not be included unless the target atom number run includes the origin atom number. Subroutine SEARC is used by this instruction, and the instruction input details are similar to those of instructions 402/412 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 $c/2$. The box dimensions must be chosen carefully so that the ATOMS array does not overflow. Vector search codes on Format No. 2 continuation cards may be used for screening if desired. (See 3.1.5.)

Columns	**Instructions 403/413 and 404/414**
3	0, 1, or 2
7-9	403, 404, 413, or 414
10-18	Org. ADR (from)
19-27	Org. ADR (to)
28-36	Tar. ANR (from)
37-45	Tar. ANR (to)
46-54	*a/2* (Å or fraction)
55-63	*b/2* (Å or fraction)
64-72	*c/2* (Å or fraction)

Columns	**Format No. 2 Continuation Card (if used)**
3	0 or 2
4-9	—
10-12	[Org. NR (from)
13-15	Org. NR (to)]
16-18	[Tar. NR (from)
19-21	Tar. NR (to)]
24	[NR type]

Columns	**Format No. 1 Continuation Card (if needed)**
3	2
7-9	—
10-18	—
27	LOGC

3.3.5.4 Instructions 405/415 and 406/416, Convoluting Sphere of Enclosure Add/Eliminate and Reiterative Convoluting Sphere of Enclosure Add/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 array. A valid origin atom must be placed in the ATOMS array with a 401, 402, 403, or 404 instruction before these instructions are used. All atoms in the ATOMS array that have atom or feature numbers within the origin number run (Org. NR) of the instruction are used as origin points of convolution. Vector search codes on Format No. 2 continuation cards may be used for screening if desired. (See 3.1.5.)

An example use for the 405 instruction is to complete the coordination shells around metal atoms without having to identify the coordination shell atoms individually. Another use might be to obtain a cluster of atoms out to the nth 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 where 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.

Instruction 406 has an added feature that makes it useful for limiting the ATOMS array to those atoms in an asymmetric unit of the unit cell. An example is the examination of electron density maps. When direct methods are used for solving crystal structures, stereoscopic drawings provide a rapid means for screening the *E* maps. If the interpolated positions of the largest peaks in the Fourier synthesis *E* map are taken as atom positions, then ORTEP can start at a given peak (usually the largest) and do a reiterative sphere-of-enclosure add to isolate a molecule if one is present. In order to terminate the convolution procedure when extraneous "bridging peaks" link the molecules, a feature has been added to the 406 instruction to prevent multiple instances of an atom (in any of its equivalent positions) from being entered in the ATOMS array. To invoke this feature, a Format No. 1 continuation card with a "1" in column 18 (ASYMUNIT) is added to the 406 instruction. The 406 instruction operates in its usual manner if the continuation card is omitted or has a "0" or blank in column 18.

Columns	**Instructions 405/415 and 406/416**
3	0, 1, or 2
7-9	405, 406, 415, or 416
10-18	Org. NR (from)
19-27	Org. NR (to)
28-36	Tar. NR (from)
37-45	Tar. NR (to)
46-54	D_{max} (Å)
63	NR type

Columns	**Format No. 2 Vector Search Code (if used)**
3	0 or 2
4-9	—
10-12	[Org. NR (from)
13-15	Org. NR (to)]
16-18	[Tar. NR (from)
19-21	Tar. NR (to)]
24	[NR type]
25-30	[D_{min} (Å)
31-36	D_{max} (Å)]

Columns	**Format No. 1 Continuation Card (if needed)**
3	2
7-9	—
18	ASYMUNIT (406 only)
27	LOGC

3.3.5.5 Instruction 410, Clear ATOMS Array

This instruction clears the ATOMS array to zero. When the program is first entered, the array is automatically set to zero.

Columns	**Instruction 410**
7-9	410

3.3.6 Orienting Instructions (500 Series)

For information on instruction 511, see Section 3.3.12.

Any Cartesian coordinate system is based on three orthonormal base vectors and an origin point. In the absence of any 500 instructions, ORTEP calculates the base vectors of the reference and working Cartesian systems (see 3.1.8) from the input cell parameters and sets the origin to (0.,0.,0.).

This series of instructions can be used to reorient the reference and working Cartesian systems. Each time the reference system is redefined or rotated, the working system is automatically made coincident with the reference system. The working system can be displaced from the reference system by rotating about the x or y axis of the reference system with a 503 instruction. The working system is always positioned from the reference system and does not depend on any previous working system orientation. After each 500 series instruction, the base vectors of the relevant Cartesian system are printed in the ORTEP output file. 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, Explicit Reference Cartesian System Assignment

Instruction 501 allows the user to define the reference Cartesian system explicitly. 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 $\mathbf{u}$ and $\mathbf{v}$. Type 1 produces base vectors that are roughly along the general triclinic coordinate axes of the crystal.

	Type 0	Type 1
Base vector 1 (x axis)	$\mathbf{u}$	$\mathbf{u}$
Base vector 2 (y axis)	$\mathbf{u} \times \mathbf{v}$	$(\mathbf{u} \times \mathbf{v}) \times \mathbf{u}$
Base vector 3 (z axis)	$\mathbf{u} \times (\mathbf{u} \times \mathbf{v})$	$\mathbf{u} \times \mathbf{v}$

The reference system x and y axes will parallel the plotter x and y axes, and the origin point ORGN will lie in the plane of the plotter. The viewer will be looking into the z axis vector of the coordinate system from the viewing distance set by the 301 instruction (see 3.3.4.1) directly above the origin point.

Columns	**Instruction 501**	Effective Primer Constant
7-9	501	—
10-18	ORGN (ADC)	000000
19-27	Vector **u** (from ADC)	155501
28-36	Vector **u** (to ADC)	165501
37-45	Vector **v** (from ADC)	155501
46-54	Vector **v** (to ADC)	156501
55-63	—	—
72	Type	1

3.3.6.2 Instruction 502, Reference Cartesian System Rotation

The crystal model can be given any desired orientation 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 by ORTEP. In addition, rotations of 120° about the body diagonal of the reference Cartesian system are permitted (achieved by a cyclic permutation of reference base vectors).

Each operation requires two fields on 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 axis of the reference system, respectively. 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 observer). 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, respectively, and the second field is blank. A -3 would rotate the structure completely around and thus not change its previous orientation. If desired, each rotation can be executed with a separate 502 instruction card.

<table>
<tr><th>Columns</th><th>Instruction 502</th></tr>
<tr><td>3</td><td>0 (or 1 if continued)</td></tr>
<tr><td>7-9</td><td>502</td></tr>
<tr><td>17-18</td><td>1, 2, 3, -1, or -2</td></tr>
<tr><td>19-27</td><td>ϕ (˚) (if value in previous field is positive)</td></tr>
<tr><td>28-36</td><td rowspan="2">[…]</td></tr>
<tr><td>37-45</td></tr>
<tr><td>46-54</td><td rowspan="2">[…]</td></tr>
<tr><td>55-63</td></tr>
</table>

3.3.6.3 Instruction 503, Working Cartesian System Rotation (Stereoscopic Rotation)

To define an orientation of the working system that is not coincident with the reference system, a 503 instruction may be used, 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. (See 3.3.6.4 and 5.4.) 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	**Instruction 503**
7-9	503
18	1 or 2
19-27	ω (°)

3.3.6.4 Instruction 504, Reference Cartesian System Origin Translation

Instruction 504 is used to translate the origin of the reference Cartesian system along the x, y, and z axes of the reference system. Stereo by translation of origin can be achieved with instruction 504, which may be used in place of the 503 instruction. However, the 504 instruction 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. (See 5.4.)

Columns	**Instruction 504**
7-9	504
10-18	Translation along x axis (in.)
19-27	Translation along y axis (in.)
28-36	Translation along z axis (in.)

3.3.6.5 Instruction 505, Reference Cartesian System Origin at Centroid

This instruction finds the first moment (i.e., centroid or center of gravity) of the atoms in the ATOMS array and makes this point the origin point (ORGN) of the reference and working coordinate systems. The base vectors of the coordinate systems are unchanged from their previous values. A weighting scheme and screening may be applied to the atoms used to calculate the centroid by using Format No. 2 trailer cards. If no trailer cards are used, all atom positions are entered with unit weights.

Columns	**Instruction 505**	Columns	**Format No. 2 Continuation Card (if used)**
3	0 or 2	3	0 or 2
7-9	505	10-12	NR (from)
		13-15	NR (to)
		24	NR type
		25-30	Weight

3.3.6.6 Instruction 506, Reference Cartesian System 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 axes of the configuration of atoms in the ATOMS array. The x axis is along the long axis of the configuration (i.e., the minimal axis of inertia) and the z axis is along the short axis of the configuration (i.e. the maximal axis of inertia). The overlap along the z-view direction is often minimized by this option. Furthermore, the xy plane is the least-squares best plane for the atomic configuration. Format No. 2 trailer cards may be used to supply weights and screening.

Columns	**Instruction 506**	Columns	**Format No. 2 Continuation Card (if used)**
3	0 or 2	3	0 or 2
7-9	506	4-9	—
		10-12	NR (from)
		13-15	NR (to)
		24	NR type
		25-30	Weight

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, 505, or 506) 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 instruction 301.

A second scaling parameter SCAL2 scales 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 listing of SCAL2 values vs. probability is given in Table 6.1. The primer constant for SCAL2 is 1.54, corresponding to 50% probability. ORTEP-III saves the user the time of looking up the SCAL2 value corresponding to a desired probability. If the value entered in columns 37-45 is a negative whole number in the range -1 to -99, it is interpreted as the probability of the ellipsoids or spheres, and the value of SCAL2 is set by the program by table lookup, using the values in Table 6.1.

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 (X0,Y0) 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.

This usually 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.

If the instruction's entry for X0, Y0, SCAL1, or SCAL2 is "0" or blank, the primer constant value is used. This means that an X0 or Y0 cannot be entered as exactly zero. If zero is wanted, a small nonzero number should be entered.

Columns	**Instruction 601**	**Instruction 602**	**Instruction 603**	**Instruction 604**	Primer Constant
7-9	601	602	603	604	—
10-18	X0	X0	—	—	8.5
19-27	Y0	Y0	—	—	5.5
28-36	SCAL1	—	SCAL1	—	1.0
37-45	SCAL2 or probability	SCAL2 or probability	SCAL2 or probability	SCAL2 or probability	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 ΔX0, ΔY0 to the previous X0, Y0 position for the ORGN placement and multiplies the existing SCAL1 by ΔSCAL1 (except if ΔSCAL1 = 0, SCAL1 is unmodified). Instruction 612 increments the position and then does an automatic scaling; 613 first increments the scale (by multiplying by ΔSCAL1*)* and then automatically repositions.

A conservative general approach is to follow a 604 with a 611 having ΔX0 = 0, ΔY0 = 0 and ΔSCAL1 = 0.9. This will simply reduce the scale 10% about the origin so that there is more space for labels, etc.

Columns	**Instruction 611**	**Instruction 612**	**Instruction 613**
7-9	611	612	613
10-18	ΔX0	ΔX0	—
19-27	ΔY0	ΔY0	—
28-36	ΔSCAL1	—	ΔSCAL1
37-45	SCAL2 or probability	SCAL2 or probability	SCAL2 or probability

3.3.8 Atom Plotting Instructions (700 Series)

These instructions produce various representations of the atom based on the familiar ball-and-stick molecular model. In the general case, the ball is an ellipsoid representing a contour surface of equal probability density of thermal motion displacement. 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 in the ATOMS array that project onto the usable part of the drawing area, defined with the 301 instruction. Atoms found to be out of bounds are bypassed, and a Fault Message (NG = 10) (see 3.4) is printed in the ORTEP output file. An atom is out of bounds under the following conditions: (1) its z coordinate in the scaled reference Cartesian system is greater than 1/2 the viewing distance, (2) its center after projection falls outside the limiting boundary of the drawing board, or (3) its projected center falls in the outermost 3/4 of the drawing margin. (See 3.3.4.1.)

An ellipsoid, for graphical purposes in ORTEP, 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 ORTEP ellipsoid are the forward principal axes, reverse principal axes, and octant-shading lines.

Fig. 3.1 shows various combinations of these elements along with the ORTEP instruction number and parameter values to produce each. It is obvious that certain of these combinations are better representations than others. Instructions 701, 702, 703, and 706 generate specific ellipsoid types as shown in Fig. 3.1. 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 may be included with each atom in the ORTEP input file. 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 for all the drawn atoms; the 900 series allows the user to position each symbol individually. The 700 series requires only three parameters as follows: (1) symbol height in inches, (2) parallel (left/right) offset in inches, and (3) perpendicular (up/down) offset in inches. The parameters refer to the model before projection, and they will change slightly during perspective projection. The parallel and perpendicular offset refer to the exact center of the six-character input field and are relative to the lettering base line set up with the 302 instruction. A symbol height of “0” or blank will cause the symbol drawing routine to be bypassed. If NPLANE = 0 in a 705/715 instruction and the symbol height is greater than zero, then chemical symbols alone are drawn on the atomic sites.

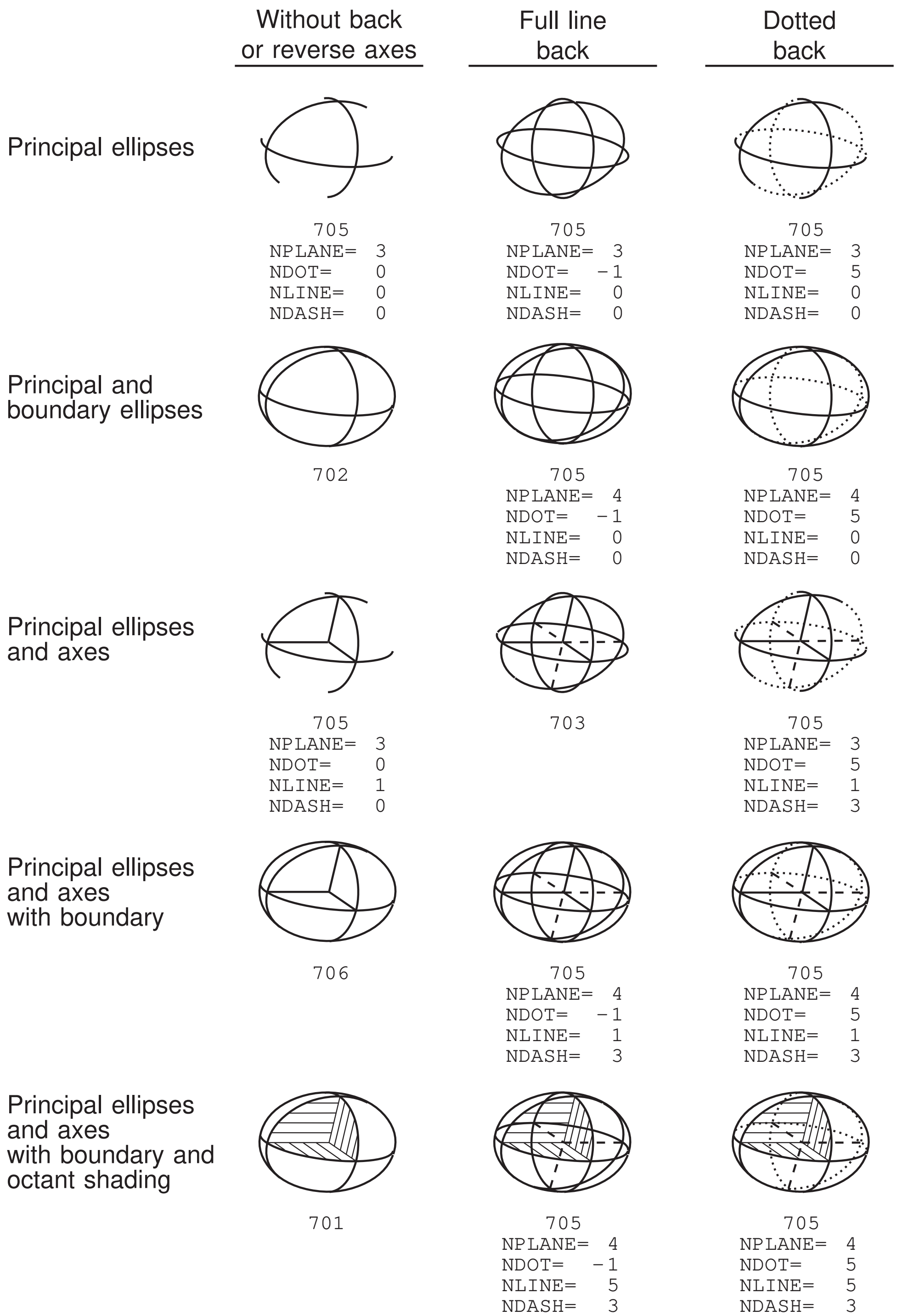

Fig. 3.1. Various combinations of ellipsoid components showing ORTEP instruction number and parameter values to produce each.

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.

Example: Assume the atoms of a 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 thick as the farthest, then ΔR(-5 in.) = 0, $\Delta R(5) = 0.008 \times (5 - 1) = 0.032$ in.; thus $A_0 = 0.016$ in. and $A_1 = 0.0032$ in.

The program widens the line by stepping radially in increments of DISP, which is set by primer constant to 0. in. A 303 instruction must be used to give DISP a positive value for this line thickening process to work.

Selected types of atoms from the ATOMS array can be drawn without having to alter the contents of the array. This is accomplished by using a number run (NR) code that 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 atom representations are used, such as for the carbon and hydrogen atoms in the cubane example. If no NR is entered, then all atoms in the array are drawn.

The ORTEP file output for the 701–706 instructions consists of the following:

- 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 the origin set by the plotter driver.

- 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).

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

- 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.

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

Instructions 711–716 are identical to 701–706 except that the 71n series suppresses all ORTEP file output except fault messages.

Columns	Instructions 701, 702, 703, 704, 706, 711, 712, 713, 714, 716	Instructions 705 and 715
3	1 (if atom selection or boundary retracing is desired; otherwise 0)	1 (if atom selection or boundary retracing is desired; otherwise 0)
7-9	701, 702, 703, 704, 706, 711, 712, 713, 714, or 716	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.)	Symbol height (in.)
55-63	Parallel offset (in.)	Parallel offset for symbols (in.)
64-72	Perpendicular offset (in.)	Perpendicular offset for symbols (in.)

Columns	Format No. 1 Parameter Continuation (if used)
10-18	[A_0 (in.)]
19-27	[A_1 (in.)]
28-36	[NR (from)
37-45	NR (to)]
54	[NR type]

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, line bonds and stick bonds. The line bond is a very crude, but rapid, method useful in drawing preliminary illustrations. It is constructed by placing the symbol ✳ on the two atom sites and drawing a single straight line between them. Line bonds are always specified implicitly.

The more elaborate bond is the stick bond, which could also be called a conical bond because of its accentuated perspective taper. (The accentuated taper may be increased or decreased by changing the value assigned to TAPER in subroutine PRIME.) Each end of the bond intersects either an ellipsoid or an enveloping cone (tangent cone) that 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 that 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 (such as produced by the 703 instruction) appear even more transparent. The radius of the stick bond and the number of lines 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 with 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 current 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 800 instructions require Format No. 2 trailer cards to provide a number of bond parameters as follows:

- Bond type (for stick bonds) 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.

- 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 semi-dimension. 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 (see 3.3.12) is used because numerical rounding may cause incorrect hidden-line elimination.

- 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.

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

- 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.

- The perpendicular offset for bond-distance regular labels (in inches) specifies the offset of the center of the distance label relative to the center of the bond.

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

Instructions 801, 802, and 803 differ from 811, 812, and 813 only in the ORTEP output file listing. The second group has no output except error messages. The first group lists: plotter coordinates in inches, scaled Cartesian coordinates (in inches) of atoms before projection, and 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 in the ORTEP output file. 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. (See 3.4.)

3.3.9.1 Explicit Bonds

Explicit stick bonds are produced with the 801/811 instructions. The bonds are described with two atom designator codes for each bond. The atom designator codes go on the 801/811 card and on Format No. 1 trailer cards if more than three atom pairs are needed. 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. As mentioned earlier, a Format No. 2 trailer card is required.

Columns	**Instructions 801/811**	Columns	**Format No. 2 Continuation Card**
3	2 (or 1 if more than 3 pairs of ADCs are needed)	3	—
7-9	801 or 811	22-24	Bond type
10-18	ADC_1 (from)	37-42	Bond radius (Å)
19-27	ADC_1 (to)	43-48	Perspective label height (in.)
28-36	[ADC_2 (from)	49-54	Perpendicular displacement (in.)
37-45	ADC_2 (to)]	55-60	Nonperspective label height (in.)
46-54	[...	61-66	Perpendicular displacement (in.)
55-63	...]	67-72	Digits indicator

3.3.9.2 Implicit Bonds

Instructions 802/812 are used for implicit stick bonds, and 803/813 are used for implicit line bonds. The symbol 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 (see 3.3.7). Number run type takes a non-zero (or non-blank) value only when working with atom “features” (see 3.1.10-12 and 4.6). At least one Format No. 2 trailer card is required.

The use of vector search code (VSC) cards for the implicit bond plotting instructions has been extended to include a provision for drawing coordination polyhedra while suppressing the unwanted bonds. In addition to describing the bond with origin and target number runs 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 array that is included in a “polyhedron” number run. This option is brought into play by a negative value in columns 43 to 48 of the VSC card.

Columns	**Instructions 802/812 and 803/813**
3	2
7-9	802 or 812
10-18	—
27	NR type

Columns	Instructions 802/812 Format No. 2 Vector Search Code: Positive value in col. 43-48	Instructions 802/812 Format No. 2 Vector Search Code: Negative value in col. 43-48	Instructions 803/813 Format No. 2 Vector Search Code: Positive value in col. 43-48	Instructions 803/813 Format No. 2 Vector Search Code: Negative value in col. 43-48
3	0 or 2	0 or 2	0 or 2	0 or 2
10-12	Org. NR (from)	Org. NR (from)	Org. NR (from)	Org. NR (from)
13-15	Org. NR (to)	Org. NR (to)	Org. NR (to)	Org. NR (to)
16-18	Tar. NR (from)	Tar. NR (from)	Tar. NR (from)	Tar. NR (from)
19-21	Tar. NR (to)	Tar. NR (to)	Tar. NR (to)	Tar. NR (to)
22-24	Bond type	Bond type	—	—
25-30	D_{min} (Å)	D_{min} (Å)	D_{min} (Å)	D_{min} (Å)
31-36	D_{max} (Å)	D_{max} (Å)	D_{max} (Å)	D_{max} (Å)
37-42	Bond radius (Å)	Bond radius (Å)	—	—
43-48	Perspective label hgt. (in.)	Polyhedron NR (from)	—	Polyhedron NR (from)
49-54	Perpendicular displacement (in.)	Polyhedron NR (to)	—	Polyhedron NR (to)
55-60	Nonperspective label hgt. (in.)	Polyhedron D_{min} (Å)	—	Polyhedron D_{min} (Å)
61-66	Perpendicular displacement (in.)	Polyhedron D_{max} (Å)	—	Polyhedron D_{max} (Å)
67-72	Digits indicator	—		

3.3.9.3 Bond Overlap

Instructions 821 and 822 are used for calculating bond/atom and bond/bond overlap rather than for drawing bonds. These are described in Section 3.3.12.

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, and bond length labels. 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, respectively, but it is often desirable to position certain labels individually with the 900 series.

ORTEP-III provides the following character set for labels:

```
ABCDEFGHIJKLMNOPQRSTUVWXYZ
abcdefghijklmnopqrstuvwxyz
0123456789—!@#$%&* () +, - ' " .
/:;<=>? space
```

General titles and bond length labels can be drawn either in perspective or parallel to the plane of the drawing (nonperspective). Chemical symbols are always drawn parallel to the plane. Instructions 913–916 produce perspective lettering, and instructions 901–906 produce regular plane lettering.

Two vectors, the upright vector and the base-line vector, are needed to describe a lettering plane. In ORTEP, 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 drawing) that is oriented with a 302 title rotation instruction (theta base line). If theta is zero, then the theta base-line vector is along the plotter positive x axis.

The exact center of the label is always referred to when specifying the position of the label. The program goes through the following steps to position the center point of the label onto the drawing.

(1) A point $P1$ is found that is either the position of atom A (columns 10-18) or the mean of two atom positions (atom A and atom B) if an atom designator exists in the atom B field (columns 19-27) of the instruction card.

(2) A point $P2$ is found by (a) translating from $P1$ along the base-line vector for the distance specified by the parallel offset and then (b) translating along the upright vector by the perpendicular offset distance.

(3) A point $P3$ is found by projecting $P2$ onto the plane of the drawing.

(4) If the *x edge reset* is greater than 0, then x is reset to this value. If *x edge reset* is less than 0, x is reset to the positive x plot boundary minus |*x edge reset*|. No resetting is done if *x edge reset* equals 0. The y parameter is handled in the same manner with *y edge reset*.

Instruction 901 produces a nonperspective atom label with theta base line, using the atom label for atom A.

A nonperspective title with theta base line is drawn with the 902 instruction. The title must be provided with the instruction on a Format No. 3 trailer card. The title should be centered about columns 36-37 of that card. However, if the title begins in column 1, it will be centered automatically (a new feature in ORTEP-III).

A nonperspective general title with normal plane lettering is produced by the 903 instruction and with perspective lettering by 913. The general vector is from atom A to atom B. The title must be provided with the instruction on a Format No. 3 trailer card. The title should be centered about columns 36-37 of that card. If the title begins in column 1, it will be centered automatically.

Instructions 904, 905, 906, 914, 915, and 916 produce bond-length labels. The first three are for nonperspective lettering with one, two, and three places after the decimal point, respectively; and the last three are for the corresponding bond-length labels with perspective. 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.

The format for the entire 900 series is as follows:

Columns	**900 Instructions**
3	0 (or 3 for 902, 903, and 913)
7-9	9*nn* (instruction number)
10-18	ADC for atom A
19-27	[ADC for atom B]
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.)

3.3.11 Save 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 1101 to start the save sequence, 1102 to terminate the save sequence, and 1103 to execute the save sequence. All instruction cards and their trailer cards between the 1101 and 1102 instructions are *executed and saved*. Each subsequent 1103 instruction then repeats all the saved instructions. There are no parameters to be entered with the 1100 series instructions.

Columns	**Instructions 1101, 1102, and 1103**
6-9	1101, 1102, or 1103

3.3.12 Overlap Correction Instructions (1001, 821, 822)

(Instruction 511 in OR TEP-II[2] has been renumbered to 1001 in ORTEP-III. Instruction 511 continues to work as it did in OR TEP-II,[2] but users should use 1001 in the future.)

Instruction 1001 activates the hidden line removal feature of ORTEP, which corrects the illustration for overlapping atoms and bonds. It stores the projected atom boundary ellipses for all atoms in the ATOMS array. It is important that the contents of the ATOMS array, the scaling and positioning, and the structure orienting parameters (controlled by the 400, 600, and 500 series of instructions, respectively) not be changed between the 1001 instruction and the drawing of the atoms and bonds by the 700 and 800 series of instructions. Otherwise, the projected outlines may be destroyed or become inappropriate.

The projected outlines of bonds are approximated as quadrangles. Those of implicitly specified bonds may be stored for overlap correction by adding Format No. 2 trailer cards to the 1001 instruction that are identical to those of the 802/812 instructions used subsequently for plotting the implicit bonds. Alternatively, implicitly specified bonds may be stored with one or more 822 instructions with the Format No. 2 trailer card set. A 1001 instruction must precede the first 822. If more than one 802/812 instruction is used to draw the bonds, there probably should be a corresponding 822 provided for each.

Explicit bonds may only be stored by using one or more 821 instructions following a 1001 instruction. These will be identical to the 801/811 instructions used subsequently for plotting the explicit bonds except for the instruction number.

As currently dimensioned, the maximum numbers of projected atoms and projected bonds that can be stored are 500 and 599, respectively. A list of the projected atoms and bonds is given in the ORTEP output file.

The projected outline information for atoms and bonds must be recalculated for each member of a stereo pair; consequently the 1001 and 821 or 822 instructions are usually the first instructions within the save sequence. The old overlap information is deleted whenever a new 500 or 600 series or 1001 instruction is executed.

All details inside atoms and bonds, including chemical symbols drawn with 700 series instructions and bond-distance labels drawn with 800 series instructions, will be corrected for overlap. Lettering drawn by the 700 and 800 series instructions that is outside the atom or bond boundaries will not be corrected for overlap unless the overlying atom or bond outline actually intersects (in projection) the atom or bond being drawn. Labels and symbols drawn with the 900 series instructions will not be corrected for overlap.

3.3.12.1 Instruction 1001, 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 (in inches) may be specified as a parameter with the 1001 instruction if desired; otherwise, the margin is set by default. The default value is calculated as follows:

for SCAL1 < 0.25: $\text{OVMRGN} = \max(0.010,\ \text{SCAL1}^{1/2} \times 0.05)$

for SCAL1 ≥ 0.25: $\text{OVMRGN} = \max(0.025,\ \text{SCAL1}^{1/2} \times 0.03)$

Some users prefer an overlap margin of 0.0 for stereoscopic drawings.

Columns	**Instruction 1001**
3	2 (if bonds are to be stored; otherwise 0)
6-9	1001
10-18	Overlap Margin 0: default value (described above) 1: 0.0 in. Value in range 0-1.0 in.
27	NR type

If the value in 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. (See 3.3.9 and 3.3.12.3.)

New on this card in ORTEP-III is the second parameter, which specifies the number run type of the number runs that follow on the Format No. 2 trailer cards.

3.3.12.2 Instruction 821, Explicit Bond Outline Storage

If explicit bonds are to be stored for the overlap correction, the attached atoms must be in the ATOMS array even though this is not a requirement for the 801/811 instructions used for plotting the explicit bonds. In general, the 821 instructions will be identical to the 801/811 instructions (except for the instruction number) used subsequently for plotting the explicit bonds. (See 3.3.9.)

3.3.12.3 Instruction 822, Implicit Bond Outline Storage

Usually, the information on implicit bond outlines is stored with the 1001 card. However, if more than 20 Format No. 2 trailer cards are needed to specify all bonds, the extra ones can be entered with this instruction. Also, 822 instructions in addition to the 1001 may be used to treat different atom features in different ways. In general, the 822 instructions will be identical to the 802/812 instructions (except for the instruction number) used subsequently for plotting the implicit bonds. (See 3.3.9.)

Columns	**Instruction 822**
3	2
7-9	822
10-18	—
27	NR type

3.3.13 Termination Instructions (Negative Series)

The -1 instruction terminates ORTEP, exiting the program via subroutine EXITNG.

The -2 instruction terminates the current structure and reinitializes ORTEP to read another structure from the same input file starting with a new title card. As many structures as desired may be cascaded in the input file in this manner before exiting with a -1 instruction. The user's initial input about the destinations for the drawing and text output hold for the entire set of structures. At the end of each structure, the user is offered the opportunity to save the drawing, view it on the screen, or edit the current instruction set before proceeding to the next structure. (See 4.1.).

Columns	**Instructions -1 and -2**
8-9	-1 or -2

3.3.14 Supplementary Instructions

The instructions available in ORTEP-III have numbers less than 1200. Any instruction in the input file with a number greater than or equal to 1200 will cause ORTEP to branch to subroutine SPARE to execute the code found there. As distributed, this is a dummy subroutine containing the single FORTRAN statement RETURN. It is provided to give users a simple way to add their own instructions without having to understand the full program logic. Subroutine SPARE has a single parameter INST, which is the instruction number.

3.4 LIST OF FAULT INDICATORS

ORTEP checks for certain errors, and when one of these occurs, an error message, "FAULT NG = *NG ADC m*" is written in the ORTEP output file. The meanings of fault indicator number *NG* is explained in Table 3.1. *ADC* and *m* identify the atom code and the instruction involved (if these are relevant). If possible, corrective measures are made by ORTEP and the calculation proceeds; otherwise, the job is terminated by calling subroutine EXITNG.

Table 3.1. ORTEP fault indicators.

NG	Subroutine Involved	Fault	Action
1	PRELIM	No sentinel found after reading 96 symmetry cards	Tries to read parameter cards
2	PRELIM	No sentinel found after reading the parameter cards for 505 atoms	Tries to read instruction cards
3	PRELIM	Anisotropic temperature factor coefficients form a matrix which is not positive definite	EXIT after printing out all rms principal values (imaginary ones are listed negative)
4	ATOM, PAXES	Symmetry operation number is higher than the number of input operations	Omit atom
5	ATOM, PAXES	Atom number is higher than the number of input atoms	Omit atom
6	EIGEN	Null temperature factor matrix or failure in bisection routine	EXIT, after printing out all principal values
7	EIGEN	Eigenvector routine failure due to null vector	EXIT, after printing out all principal values
8	INITSC	Error initializing screen driver	EXIT
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, SEARC	Insufficient number of atoms in ATOMS array	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 array is full	Omit all succeeding atoms
17	LAP700, LAPAB	Maximum number of projected ellipses (20) over an atom or bond to be drawn exceeded	Additional ellipses not corrected for overlap
18	LAP800, LAPAB	Maximum number of quadrangles (30) over an atom or bond to be drawn exceeded	Additional quadrangles (bonds) not corrected for overlap