APPENDIX B

GLOSSARY OF VARIABLES IN ORTEP-III COMMONS

*	UNNAMED	Main Common Block
	A(9)	Direct crystal cell parameters, a, b, c, cos α, cos β, cos γ, α, β, γ.
	AA(3,3)	Metric tensor **g** where $\mathbf{g}_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.
	AAREV(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the reference Cartesian system. **AAREV = AA REFV.**
	AAWRK(3,3)	Postfactor transformation matrix to convert coordinates from triclinic to the working Cartesian system. **AAWRK = AA WRKV**.
	AID(3,3)	Identity matrix.
	REAL*8 AIN(140)	Array containing the input parameters of the current ORTEP instruction.
	REAL*8 ATOMID(500)	Atom designator codes of atoms in ATOMS array.
	ATOMS(3,500)	Temporary storage of atom coordinates in any of several coordinate systems.
	BB(3,3)	Reciprocal metric tensor. $\mathbf{BB} = \mathbf{AA}^{-1}$.
P	BRDR	Border (margin) width in inches extending inward from plot boundary.
	CD(8,20)	Holds the real values entered on a Format No. 2 trailer card. Used in conjunction with KD array.
P	CONT(5)	Constants used in subroutine RADIAL.
	D(3,130)	Array in which three-dimensional points on an ellipse are stored by RADIAL.
	DA(3,3)	Transmits conjugate vectors to RADIAL. Also used for temporary storage.
P	DISP	Displacement parameter for retracing.
	DP(2,130)	Array in which two-dimensional points for ellipse are stored after projection.
	EDGE	Distance in inches from a projected point to the closest boundary. Set in PLTXY.

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(3,3,96)	Rotation matrices for input symmetry operators based on triclinic system. Used with TS array.
	IN	Logical unit number of input file.
P	ITILT	Indicator used to signal subroutine DRAW, whether or not to do perspective labeling.
	KD(5,20)	Holds the integer values entered on a Format No. 2 trailer card. Used in conjunction with CD.
P	LATM	Number of entries in ATOMS array.
	NATOM	Number of input atoms.
P	NCD	Number of Format No. 2 trailer cards for an instruction.
P	NG	Fault Indicator value.
	NJ	Instruction number/100.
	NJ2	Last two decimal digits of the instruction number (instruction = NJ $\times$ 100 + NJ2).
	NOUT	Logical unit number of text output file.
	NSR	Logical unit number of scratch file.
	NSYM	Number of input symmetry operators.
P	ORGN(3)	Triclinic coordinates for the atom that is the origin of the drawing (i.e., on the optic axis for the projection).
	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. $\mathbf{REFV}^{T} = \mathbf{AAREV}^{-1}$.
P	`RES(4)`	Regulates the resolution of the plotting of a given ellipse as a function of the longest principal axis x in the given ellipsoid of the scaled model. $x \geq$ RES(1) — 128-point ellipse RES(1) > $x \geq$ RES(2) — 64-point ellipse RES(2) > $x \geq$ RES(3) — 32-point ellipse RES(3) > x — 16-point ellipse RES(4) — 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 that sets the ellipsoid scale relative to SCAL1.
P	`SCL`	SCL = SCAL1 × 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|.
P	`THETA`	Angle in degrees between plot x axis and lettering base-line vector.
	`CHARACTER*4 TITLE(18)`	Alphanumeric job title storage.
	`CHARACTER*4 TITLE2(18)`	Alphanumeric information storage for Format No. 3 trailer card.
	`TS(3,96)`	Translation vector for each input symmetry operator. 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),V3(3),V4(3), V5(3),V6(3)	Temporary storage.
	WRKV(3,3)	Same definition as for REFV except that this one is for working Cartesian system. $\mathbf{WRKV}^T = \mathbf{AAWRK}^{-1}$.
P	XLNG(3)	Elements 1 and 2 are *x* and *y* plot dimensions. Element 3 is not used.
P	XO(3)	Elements 1 and 2 denote the position in plotter coordinates (in inches) where ORGN is placed. Element 3 is used to transfer *z* coordinates to subroutine DRAW when perspective lettering is used.
	XT(3)	Triclinic coordinates for an atom position are placed here by subroutine XYZ.
	DFL	**Default Values for User Input**
	CHARACTER*60 ATOMFI	Default name of file containing atom parameters used by subroutine READIN.
	CHARACTER*4 EXT	Default filename extension for ORTEP output.
	FPAPLEN	Default page length for drawing
	IDRAW	Default drawing destination indicator.
	CHARACTER*60 INFILE	Default input file name.
	IORIENT	Default orientation of drawing
	IOUT	Default ORTEP text output logical unit number.
	NS	**Output Drawing Parameters**
	NDRAW	ORTEP drawing destination indicator. NDRAW=0: none NDRAW=1: screen NDRAW=2: Postscript file NDRAW=3: HPGL file NDRAW=9: Reserved for future use
	NORIENT	Orientation of drawing.
	NPF	Logical unit number of drawing output file.
	NVAR	Temporary storage.
	OLAP	**Overlap Correction Variables**
	CONIC(7,500)	Overlap correction ellipses describing intersection of enveloping cones with drawing plane.

	COVER(6,20)	Stores up to 20 overlapping ellipses for an atom or bond being drawn.
	KC(20)	Which ellipses overlap the atom or bond being drawn.
	KQ(30)	Which quadrangles overlap the atom or bond being drawn.
	NCONIC	Total number of projected ellipses stored for overlap calculations.
	NCOVER	Number of projected ellipses over an atom or bond to be drawn.
	NQOVER	Number of quadrangles over an atom or bond to be drawn.
	NQUAD	Total number or projected bond quadrangles for overlap calculations.
	OVMRGN	Overlapping element margin.
	QOVER(3,4,30)	Stores up to 30 overlapping bond quadrangles for atom or bond being drawn.
	QUAD(9,600)	Overlap correction bond quadrangles projected onto drawing plane.
	SEGM(50,2)	Visible segments of an ellipsoid or bond element to be drawn.
	PARMS	**Input Atom Parameters**
	CHARACTER*8 CHEM(505)	Names for input atoms.
	EV(3,505)	Root-mean-square displacements for each principal axis of each input atom.
	INTEGER*2 IDENT(2,505)	Two feature identifiers for each input atom.
P	MAXATM	Array size for input atoms. (Currently 505.)
	P(3,505)	Triclinic positional coordinates for the input atoms.
	PA(3,3,505)	Matrices for each input atom made up of three orthogonal column eigenvectors each 1 Å long, based on the triclinic system (principal axis vectors).
	PS	**Encapsulated Postscript Output Parameters**
	IXMIN	Minimum x value of illustration.
	IXMAX	Maximum x value of illustration.

	IYMIN	Minimum y value of illustration.
	IYMAX	Maximum y value of illustration.
	IXT	Page translation along x.
	IYT	Page translation along y.
	QUEUE	**Editor Variables**
	CHARACTER*73 HQUE(96)	Original instruction set as read from input file.
	CHARACTER*73 INQ	Next instruction held in memory to be processed.
	NBACK	Number of lines in original instruction set as read from input file.
	NED	Logical unit number of temporary file used by editor.
	NEXT	Line number of next instruction held in memory to be processed.
	NQUE	Current number of instruction lines held in memory.
	CHARACTER*73 QUE(96)	Instruction lines held in memory.
	TRFAC	**Plot Translation Factors**
	XTRANS	Shift of plot origin along x-axis.
	YTRANS	Shift of plot origin along y-axis.

*Letter "P" indicates Prime Parameter (i.e., initialized in subroutine PRIME).