Chapter 8.2

Ortep-3 for Windows

Version 1.08

A current version of ***Ortep-3 for Windows*** is available from the Web-site
http://www.chem.gla.ac.uk/~louis/software/ortep3

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1. INTRODUCTION

Ortep-3 for Windows is a version of the current release of ORTEP-III (1.0.3), which incorporates a Graphical User Interface (GUI) to make the production of thermal ellipsoid plots much easier. Most of the commonly used features of ORTEP-III are directly available from the GUI, and all the facilities present in ORTEP-III are also available in ***Ortep-3 for Windows***. The main features are:

- ***Ortep-3 for Windows*** can directly read many of the common crystallographic ASCII file formats which hold information on the anisotropic displacement parameters. Currently supported formats are SHELX, GX, CIF, SPF, CRYSTALS, CSSR-XR, CSD-FDAT, GSAS, Sybyl MOL, XYZ, PDB, Rietica-LHPM and FULLPROF. In addition, ***Ortep-3 for Windows*** will accept any legal ORTEP-III instruction file.
- Up to 500 atoms may be present in the asymmetric unit, and up to 1999 atoms may be drawn. Covalent radii for the first 94 elements are stored internally, and may be modified by the user. All bonds are calculated automatically, based on these covalent radii. Any individual bonds may be selected for removal, or for a special representation.
- Several style-templates are supplied, but the graphical representations of thermal ellipsoids for any element or selected sets of atoms can be individually set. All the possible graphical representations of thermal ellipsoids in ORTEP-III are also available in ***Ortep-3 for Windows.*** Over 120 different colours are stored internally and up to 200 colours may be defined. All graphic objects may be drawn in any colour.
- A mouse labelling routine is provided by the GUI. Any number of selected atoms may be labelled, and any available Windows font may be used for the labels. The font attributes, *e.g.* italic, bold, colour, point-size *etc* can also be selected via a standard Windows dialog box.
- The HPGL and PostScript Graphics drivers from ORTEP-III provide standard graphic metafiles, and it is also possible to get high quality graphics output by printing directly to an attached printer. The screen display may be saved as BMP metafiles, and may also be copied to the clip-board for subsequent use by other Windows programs, e.g. word processing or graphics processing programs. Colour is available for all these output modes.
- Ray-traced output is available using the Raster3d or POV-Ray formats. Several representations are available from the POV-Ray interface, including thermal ellipsoids (standard ORTEP, RMSD and MSD surfaces) and van der Waals plots.
- A simple text-editor is provided, so that input files may be modified without leaving the program. The ORTEP-III instruction file which is written by the GUI (and which corresponds to the currently displayed picture) may be saved at any time for future use or modification.
- Symmetry expansion of the asymmetric unit to give complete connected fragments may be carried out automatically, or the user may define a single seed-atom for symmetry expansion of a single fragment.
- Unit cell packing diagrams are produced automatically.
- A number of options are provided to control the view direction. The molecular view may be rotated or translated by button commands from the tool bar, and views normal to crystallographic planes may also be obtained.

2. HOW *ORTEP-3 FOR WINDOWS* WORKS

Ortep-3 for Windows uses the current release of ORTEP-III (version 1.0.3 of January 2000 by Carroll K. Johnson and M. N. Burnett, ORNL-6895) as the drawing engine, with very little change. Some of the arrays have been increased in size, and some features which are rendered redundant by the GUI (*e.g.* the line editor, graphics routines and command line menus) have been removed.

Major features of the GUI, over and above those provided in ORTEP-III itself, are the mouse labelling routine (see **5.4.2**), interactive GEOM (see **5.8.4**), and some extra output facilities (see **5.1.6**, **5.1.7**, **5.6.6** - **5.6.8**). The GUI is essentially an editor which writes input files for ORTEP-III. The GUI makes production of ORTEP pictures substantially easier than by using a standard instruction set to ORTEP-III. In most instances it not necessary for the user to understand how ORTEP-III works, although if some of its less common features are required, *e.g.* the drawing of critical net illustrations, then it will be necessary to prepare an ORTEP-III instruction file (or modify one produced by ***Ortep-3 for Windows***). *Users should be aware however that the program* ORTEP-III *requires FORTRAN fixed format instructions, and any format error in the instruction file may result in a program crash or obscure failure.* The full ORTEP-III manual may be obtained from the Web site:

http://www.ornl.gov/ortep/ortep.html

Each drawing of a new structure is initiated by opening a new coordinate file (from the **FILE** menu item). Opening a new file has the following results:

- The selected coordinate file is copied to an internal temporary file. This file is then checked (by a unsophisticated routine!) for the file-format. The decision as to the file-format is made on the basis of the *contents* of the file, rather than the filename extension. For instance, if TITL and FVAR instruction cards are found in the file, then it is assumed to be a SHELX file, regardless of the file extension. If there is an error in reading the file, or if the program does not recognise the file format, a message to this effect is issued from the status bar (see p. 7), and the program is ready to read another coordinate file.
- If the coordinate file is successfully read, then the style is reset to the default style **Organic**, the contents mode is set to **Use Asymmetric Unit**, and a number of other options are reset to their standard conditions.
- If the selected coordinate file is NOT an ORTEP-III instruction file, the program then writes its own internal ORTEP-III instruction file which is subsequently interpreted by ORTEP-III and displayed on-screen. All facilities of the GUI are then available to modify the ORTEP picture. Once a suitable view is obtained, hardcopy graphic output may be produced in a number of ways.
- On the other hand, if the selected coordinate file is an ORTEP-III instruction file, the user is offered a choice. The file may be treated as the other coordinate file formats, with all the ORTEP drawing instructions being ignored. Alternatively, the file may also be interpreted *directly*. If this latter option is chosen, then most of the facilities of the GUI are by-passed, the only ones available being the PostScript and HPGL metafile output (**FILE** menu), the mouse labelling routine (**LABELS** menu) and all items from the **GRAPHICS** menu. Note that ORTEP-III is downwards compatible, and will accept instructions from previous versions of ORTEP.

3. ORTEP PARAMETERS

Many of the parameters required by the GUI and ORTEP-III have sensible default values embedded in the program. These values may be modified dynamically by selecting the menu item **Change ORTEP Parameters** in the **STYLES** menu (see **5.3.2)**. A parameter box is then displayed, which allows the user to scan all the modifiable parameters and enter any new desired value. Changes made in this way are not stored permanently. Alternatively, the ORTEP3.INI file may be modified so that the new values are used whenever the program is loaded (see **4.10**). A full listing of all the **ORTEP Parameters** is given in Table 1 at the end of this manual.

4. GENERAL INFORMATION ON *ORTEP-3 FOR WINDOWS*

The maximum number of atoms in the asymmetric unit is 500, while the number of atoms which may be drawn has been increased to 1999 in ***Ortep-3 for Windows*** so that unit cell packing diagrams are more complete. The program ORTEP is primarily designed for drawing publication quality thermal ellipsoid plots of small molecules. It is relatively slow, and not really suited to drawing macromolecular structures (there are many other excellent packages which do this). Nor is it really a "visualisation tool" for crystallographic analysis, though it has facilities which allow it to be used in this fashion.

Information on the new features in versions since 1.05 is given in the Help-HypertextHelp menu item. These changes are generally of a minor nature, and the information in this manual is still valid.

4.1 ATOM LABELS

While ***Ortep3 for Windows*** does not explicitly prescribe any format for atom labels, it is *strongly recommended* that the atomic label should consist of the chemical symbol followed by a character string where at least the first character is an non-alphabetical character (preferably an integer representation). The character string may optionally be enclosed in brackets. The atom label is used to determine the atomic type for several of the input formats, where this information is not obtainable in another way.

It is also very important that each atom has a unique label. All labels are checked when the coordinate file is read, and if any duplicate labels are found, a warning is issued. Several of the mouse-selection options will not be available in this case. A label can have a maximum of 8 characters.

4.2 BONDS

Bonds are automatically calculated in ***Ortep-3 for Windows*** using the stored covalent radii. A bond is considered to exist between two atoms if the distance between them is greater than the ORTEP parameter **BondSearchDistanceMin** and less than the sum of their covalent radii plus the ORTEP parameter **BondToleranceFactor**. The ORTEP parameter **BondSearchDistanceMax** defines the upper limit for any possible bond distance. The internally stored covalent radii for elements may be modified using the **Set Element Style**

menu item in the **STYLES** menu, and the three ORTEP parameters may be modified in the normal fashion (see page 6). A judicious choice of the values for these parameters should allow unusually long or short bonds to be displayed, or not displayed, as required.

By default, all bonds (except those to H atoms) are drawn with the same "standard" style. This style may be altered using the menu item **Set Bond Style**. In addition, individual bonds, or sets of bonds, may be given a special style or may be eliminated from the illustration altogether, using the menu items **Selected Bond Style** and **Delete Selected Bond** respectively.

4.3 COLOURS

Ortep-3 for Windows allows a large choice of colours. Over 120 colour names and RGB triplet values are stored internally, see Table 2. The exact appearance of these colours will depend on the colour-depth of your monitor, which should be at least 256 colours. The use of 16-bit colour or better is recommended. Note that case is important in declaring colour names, *e.g.* "SkyBlue" is not the same as "Skyblue". Additional colours may be defined (or re-defined) in the file RGBCOLS.DEF, which is located in the *home directory* (see **4.11**). The previous limitation on the number of colours which could be displayed has now been removed, and graphic objects may be drawn in any colour The colour tool-button (see **4.8**) switches between colour and monochrome modes.

4.4 ERROR MESSAGES AND STATUS BAR

Error messages from ***Ortep-3 for Windows*** are usually provided via the status bar. The default position of the status bar at the bottom of the screen may be altered with the ORTEP Parameter **StatusBarPosition** in the ORTEP3.INI file (see Section **4.10**). These messages are left on screen for a few seconds, to allow the user time to read them. The length of time the message is left on screen can be changed by modifying the ORTEP parameter **MessageDelay**. In some instances a message box is displayed.

4.5 MENU ITEMS

Many of the menu items in ***Ortep-3 for Windows*** are toggles or are ganged. If several menu items are ganged, they form an exclusive set of options, of which only one may be active at any time. If a toggled or ganged menu option is active, this is indicated by a check (√) mark in front of that item. For instance, if the user wishes to have brackets around the atomic labels, then the **Brackets on Labels** menu item from the **LABELS** menu must be selected. Once this is done, this item will become active and have a check mark in front. If a coordinate file is already loaded, a new picture will then be drawn, with brackets round all labels. If the user wishes to remove these brackets, the **Brackets on Labels** menu item must be clicked again, causing the control to become inactive.

4.6 MOUSE SELECTION AND LABELLING OF ATOMS

Several menu items rely on selection of atoms by using left mouse-button clicks. In this case, an OK/CANCEL box will appear in the bottom left corner of the graphics region.

WHEN THIS BOX IS DISPLAYED, ALL OTHER MENU ITEMS ARE INOPERATIVE.

The actions of the OK and CANCEL buttons depend on the specific routine, and are given by a message in the status bar. A right mouse-button click has the same effect as clicking the OK

button. In general, when an atom is selected, a red (or blue) dot will appear at the atomic centre, and the name of the atom will be displayed in the status bar. The routine finds the *nearest* atom to the clicked position, so that if two or more atoms are close together or superimposed, the user may inadvertently select the wrong atom. It is usually possible to reverse an incorrect selection. If duplicate atom names are found, then many of the mouse selection options are unavailable. This is because the name is used in the search routines.

The mouse labelling routine in ***Ortep-3 for Windows*** is a service provided by the GUI (see **5.4.2**) and is independent of ORTEP-III. There are two types of font available for the mouse labels, the font supplied by the GUI (the Graphics font), and the font embedded in ORTEP-III itself (hereafter called the ORTEP font). The choice of which to use is basically a cosmetic one. If PostScript or HPGL files are to be written, then only a limited set of fonts are available. If the graphics screen is directly printed, then either font may be used. The characteristics of each are:

- ***ORTEP font:*** There is only one character set available (see ORTEP-III manual for details). The size of characters and the colour of the font may be altered using the **Select Graphics Font** menu item in the same was as the GUI font. *If this font is used, the symmetry adapted labelling (see last paragraph of **5.4.2**) is NOT available for technical reasons.*
- ***GUI (or Graphics) font:*** Any available Windows font may be used. The font size and other attributes are set by the FONT dialogue box obtained from the **Select Graphics Font** menu item (under **Graphics** menu). These Windows fonts are not available for Postscript or HPGL output, or saved ORTEPxxx.INS files.

4.7 SYMMETRY OPERATORS

Unlike most crystallographic programs, ORTEP-III does not automatically take into account either lattice centring or centres of symmetry, so these operators must either be included implicitly in the asymmetric unit, or as explicit symmetry operators in the ORTEP-III file written by the GUI. No more than 96 symmetry operators are allowed in ORTEP-III, this number being sufficient to cover the multiplicity of the general site for all *except* the following four cubic space groups:

Fm-3*m* (225), *Fm*-3*c* (226), *Fd*-3*m* (227) and *Fd*-3*c* (228)

for which this number is 192. The program ***Ortep-3 for Windows*** automatically expands the symmetry operations given in the input coordinate file to include explicitly any lattice centring or centre of symmetry. In general, an input coordinate file will only include the unique symmetry operations (*i.e.* not those related by a lattice translation or inversion centre). The CIF format is unusual in that it requires ALL symmetry operators to be present. The order of the symmetry operations generated by **Ortep3 for Windows** is as follows:

(i) the unique symmetry operators from the input file (including identity operator), in the given order
(ii) if the structure is centric, the centrosymmetrically related operators, in the same order as (i)
iii) if not primitive then lattice translations for all operators in (i) {and (ii) if present} are added. For *F*-centred lattices, the order of added lattice translations is (1/2,1/2,0) then (1/2,0,1/2) then (0,1/2,1/2).

The symmetry operators used by ***Ortep-3 for Windows*** may be displayed using the menu item **List Symmops** in the **CALCULATE** menu (see **5.8.3**). In the present version, if the input file

is of CIF format, then only the first 96 symmetry operators are accepted. If the CIF format is used for any of the above four space groups, then it is suggested that the lattice type is declared as Primitive, and all the lattice translations are included explicitly in the asymmetric unit. Symmetry operators relating to the F-lattice translations should then be removed.

4.8 TOOL BAR and TOOLS

A number of operations are provided by the tool-bar above the graphics screen. There is a help facility on all of these (with a somewhat arbitrary time delay) to explain their purpose. All rotations and translations are provided by this tool bar. The default rotation increment angle is 10^{o} but this may be altered. Two general operations are also available from mouse clicks on the graphics window :

- a left mouse click near an atom will display that atom name, position and thermal parameter(s) in the status window.
- a right mouse click will bring up the ORTEP QUICK MENU as a pop-up menu. This allows the user to modify easily some commonly used parameters such as ellipsoid probablity.

4.9 HARD COPY GRAPHICS OUTPUT

There are two methods of obtaining hardcopy output from ***Ortep-3 for Windows***, either as standard graphic metafiles in HPGL and PostScript format (**Write HPGL File** and **Write PostScript File** see Section **5.1.4**), or by saving the graphics screen in various ways (see Sections **5.6.6** - **5.6.8**). Full details of both methods are given in these Sections. The ORTEP parameter **PlotLineWidthA4/DJS** controls the drawn linewidth for the HPGL, PostScript and **PrintGraphicsScreen** options. The default values give a good solid line. The corresponding parameter for the graphics screen is **ScreenLineWidth**, and this parameter is also used for the direct screen copies, *i.e.* **Copy To Clipboard** and **Export BMP.**

There is now also an interface from ***Ortep-3 for Windows*** to the rendering packages Raster3D and POV-Ray. The latter in particular can provide excellent presentation quality graphical images. See Sections **5.1.6** and **5.1.7**.

4.10 CUSTOMISATION OF ORTEP-3 FOR WINDOWS

There are a number of ways of customising the defaults in ***Ortep-3 for Windows***. This can be carried out dynamically (see p. 6), but if the user finds that a different default is normally required, then a better way is to modify the values in the ORTEP3.INI file, which is found in the same directory as the program executable. All the ORTEP parameters may be changed in this way. The character set for the representations of the 96 symmetry operators can also be changed in this way. Multiple entries of **SymmLabelCharSet** will be read from the ORTEP3.INI file. Any number of one- or two-character arguments (separated by blanks) may be entered on each line (of up to 80 characters) until a maximum of 96 symbols have been entered. Any further entries are ignored. If a **SymmLabelCharSet** entry has no arguments, then ALL 96 operator symbols will be set to a blank (this deactivates the automatic addition of symmop symbols, see **5.4.6**).

For example, the following line added to the ORTEP3.INI file will have the effect of setting the first 10 of the symmop symbols to the letters “b” - “k” (the symbol “a” will never be used but is essential in the list).

SymmLabelCharSet=a b c d e f g h i j k

See Table 1 for full details of all **ORTEP Parameters.**

4.11 SYSTEM FILES AND DIRECTORIES

There are two directories used by ***Ortep-3 for Windows***, the *home directory* and the *working directory*. The home directory is where the program executable ORTEP3.EXE and system files ORTEP3.INI, RGBCOLS.DEF and ATOMCOLS.DEF are located. On first loading ***Ortep-3 for Windows***, the environment variable **ORTEP3DIR** is examined. This must be set to the home directory path: if it is not set, the program will halt. Generally, the best way to set this environment variable is by adding the following line to your AUTOEXEC.BAT file:

set ORTEP3DIR=*home_directory_fullpathname* *e.g.* set ORTEP3DIR=c:\ortep3

There are two ASCII output files which are written by ***Ortep-3 for Windows***, ORTEP.LST (the listing file from ORTEP-III) and ORTEP.INS (the ORTEP-III instruction file written by the GUI). They are usually of little interest, and are written to the home directory, where they will consequently always be overwritten. If there is an unexpected failure however, these files may be examined.

All other files written by ***Ortep-3 for Windows*** will be placed in the *working directory*, the same directory as the current coordinate file.

5. FULL DETAILS OF THE GUI FACILITIES

5.1. FILE MENU

5.1.1 Open Coordinate File

As explained above, this menu item must be selected when a new structure file is to be input. The routine performs a simple check on the contents of the selected file, to determine the file-format, and hence the subsequent action to be taken. The following common crystallographic coordinate file-formats are currently supported: SHELX, GX, CIF, SPF, CRYSTALS, CSSR-XR, CSD-FDAT, Sybyl MOL, XYZ, Rietica-LHPM and FULLPROF. The file extension is NOT used in this check, so that the filters given in the **Select Molecular Coordinate File** dialog box are for guidance only, and indicate the most common extensions given for these file types.

Regardless of the file-format, only the first 500 atoms read are stored by ***Ortep-3 for Windows***, any extra ones being ignored. If no atoms are found in the file, the program issues a message to this effect at the status bar. All file-formats are read automatically, but if there is a failure, the user may find the following information useful in tracking down the source of the problem. If there is a simple syntax error in the input file, the **Ortep Text Editor** may be used to modify this file without leaving ***Ortep-3 for Windows***. After editing is finished, the **Open Coordinate File** menu item will need to be re-selected.

5.1.1.1 SHELX format file.

The presence of the **TITL** and **FVAR** instructions trigger the recognition of a SHELX file. The following instructions, with the correct information, are ESSENTIAL for success in reading a SHELX file.

TITL

CELL lambda (not used) a,b,c,alpha,beta,gamma

SFAC

UNIT

LATT

SYMM

FVAR

Atom cards

All other legal SHELX instructions are ignored.

5.1.1.2 GX format file.

The presence of the **TITLE** and **CONTENTS** instructions trigger the recognition of a GX file. The following instructions, with the correct information, are ESSENTIAL for success in reading a GX file.

TITLE

CELL a,b,c,alpha,beta,gamma

CONTENTS (at least one element type)

LATT (if not centrosymmetric and primitive)

SYMM (if not triclinic)

ATOM cards

All other legal GX instructions are ignored

5.1.1.3 CIF format file.

The presence of a DATA_ statement triggers recognition of a CIF file-format. The following data items are ESSENTIAL (in each data_ block) for success in reading a CIF file. Note that the CIF format requires that all symmetry operators are explicitly given (including lattice translations and centres of symmetry).

data_
_cell_length_a
_cell_length_b
_cell_length_c
_cell_angle_alpha (if missing 90^o assumed)
_cell_angle_beta (if missing 90^o assumed)
_cell_angle_gamma (if missing 90^o assumed)
_symmetry_equiv_pos_as_xyz (if missing space group *P*1 assumed)

a loop with the following data

_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

and possibly

_atom_site_type_symbol
_atom_site_U_iso_or_equiv

PLUS another loop containing the data items (if **_atom_site_U_iso_or_equiv** is not present. If no U^{ij} information is present, a default U_{iso} of 0.05 $Å^2$ is assumed)

_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12

The following data item will also be used, but is not mandatory.

_atom_type_symbol

All other (standard or non-standard) CIF data items are ignored. Any logical error in the construction of the CIF (as detected by the input routines of CIFTBX) will immediately terminate input. Any CIF file written by SHELX or PLATON should be suitable for ***Ortep-3 for Windows***.

5.1.1.4 SPF (PLATON/PLUTON) format file.

The presence of a **TITL** and **ATOM** plus any of the **UIJ**/**BIJ**/**U**/**B** instructions trigger the recognition of an SPF file. It is vital that the **ATOM** instruction *precedes* the corresponding thermal parameter **UIJ**/**BIJ**/**U**/**B** instructions for each individual atom. The following instructions are ESSENTIAL for success in reading an SPF file.

TITL

CELL (wavelength) a,b,c,alpha,beta,gamma

LATT (if absent P C - primitive, centrosymmetric - assumed)

SYMM (if not triclinic)

ATOM

and one of the following for each **ATOM** card

UIJ or **BIJ** or **U** or **B**

5.1.1.5 CSD-FDAT format file.

A successful decoding of the first line in the file will trigger the recognition of a CSD-FDAT file. All structures will be extracted, and the user will then be presented with a dialog box to select the structure to display. In the current version of ***Ortep-3 for Windows*** only one structure may be selected for viewing at any one time.

5.1.1.6 CSSR-XR format file.

A successful decoding of the first line in the file will trigger the recognition of a CSSR-XR file.

5.1.1.7 GSAS format file.

A successful search of contents of the file will trigger the recognition of a GSAS file. In the current version, only information on the *first* phase is extracted.

5.1.1.8 CRYSTALS format files.

The presence of a READ instruction triggers the recognition of a CRYSTALS LIST-5 format file. The LIST 1 and LIST 2 unit cell and space group/symmetry operator files are also required. These should be concatenated into the LIST 5 file.

The following data are ESSENTIAL.

REAL a,b,c plus **all angles** OR any angle not 90. degrees (in the latter case keywords are essential *e.g.* **BETA=110.5**). At present the reciprocal cell cannot be used.

If the lattice type is noncentrosymmetric and/or is not primitive then:

CELL LATTICE = (*e.g.* **F**) , **CENTRIC=NO**

If not triclinic then:

SYM cards (NOTE: the identity operator is not required, but will be ignored if present)

All other data items, apart from **ATOM** cards (and any of their **CONTINUE** cards, if present) will be ignored.

5.1.1.9 ORTEP format files.

Ortep3 for Windows will read any ORTEP instruction file. The user is offered two choices when reading this format. The ORTEP drawing instructions may be interpreted directly, effectively by-passing the GUI. Alternatively, the user may extract just the crystallographic information from the file, and ignore all ORTEP drawing instructions. In the latter case, the full facilities of the GUI are available, but it is *very important* that the atom labels in the ORTEP file follow the recommendations outlined in **4.1**. Any blank or uninterpretable labels will result in that atom being ignored.

5.1.1.10 Sybyl MOL format files.

A successful decoding of the file will trigger recognition of a Sybyl MOL format file. The first line should contain the number of atoms and the word “MOL” in Fortran format (i4,1x,a3). Since no anisotropic displacement parameters are available, the default style for this format is PLUTO.

5.1.1.11 XYZ Angstrom coordinate format files.

A successful decoding of the file will trigger recognition of an XYZ Angstrom coordinate format file. There should be two header lines before the atomic coordinates. Either of these should contain a single entry in free format, the integer number of atoms. The content of the other line is immaterial, but should not be blank. If two lines containing a single integer are found, the second one is used. If the number of atoms found does not tally with this number, an error is assumed. The atom coordinates should be entered one on each line, and will be read in free format. The first field should either be a character string representing the element type, or an integer representing the atomic number. The remaining three fields should contain the Angstrom coordinates. A cubic unit cell of 1 Å is assumed. Since no anisotropic displacement parameters are available, the default style for this format is PLUTO.

5.1.1.12 Rietica-LHPM and FULLPROF format files.

A successful decoding of the file will trigger recognition of these two formats commonly used for powder diffraction/Riteveld analysis. They have not been as extensively tested as the other formats and some problems may remain.

5.1.1.13 Brookhaven PDB format files.

A successful decoding of the file will trigger recognition of the PDB format. The only data interpreted are those on the ATOM, HETATM and ANISOU cards, all other cards are ignored. The atom naming scheme is important since an unrecognised atomic type will cause this routine to fail. This input is NOT intended for real protein structures (ORTEP is limited to 500 atoms) but it it now a commonly used format for small molecules and hence included in ***Ortep-3 for Windows***.

5.1.2 Edit Coordinate File

A simple text editor is provided in **Ortep3 for Windows** so that the input file may be edited without leaving the program. Although there are facilities in the GUI for omitting specified atoms, it is often simpler and less frustrating to prepare an input file which only contains the atoms required. For instance, when only *some* of a set of symmetry equivalent atoms are required, there is no option but to prepare an edited input file, since the **Exclude Selected Atom** and **Delete Bond** routines in the present version of ***Ortep-3 for Windows*** will remove ALL symmetry equivalents. The usual Cut, Paste, Copy, and cursor-insertion editor functions are provided. Naturally, this editor may be used for any text file.

5.1.3 Save ORTEP3 file

Selecting this menu item will save the current ORTEP-III instruction set to a file called ORTEPxxx.INS where xxx varies from 001 to 999. This will be written into the current working directory. Previous versions will not be overwritten. If **the Mouse Labelling** option is active, then labels will be written to the file. **NOTE** that this file is NOT compatible with the standard release of ORTEP-III (mainly because a much larger number of trailer cards are allowed in ***Ortep-3 for Windows***).

5.1.4 Write HPGL File/ PostScript File

Selecting these menu items will write an HPGL or PostScript format metafile, corresponding to the currently displayed picture. The file is written to the current working directory, and is called ORTEPxxx.HPG or ORTEPxxx.EPS (xxx ranging from 001 to 999). Previous HPGL or PostScriptfiles written by ***Ortep-3 for Windows*** will not be overwritten. If the option **Mouse Labelling** is active, then atom labels close to the positions shown on the screen display will be also drawn. If the **Underscore on Labels** option (see **5.4.4**) is *NOT active* and the **Mouse Labels (GUI font)** is active, then the symmetry indicator characters will be drawn as *superscripts* The user may choose to write either black & white or colour HPGL or PostScript files. The background colour for PostScript and HPGL files is ALWAYS white, and any graphical object drawn in white on screen (*e.g.* bonds) will be drawn as black in the PostScript file.

5.1.5 Write SHELX File / XYZ File

The atomic contents of the screen *as currently displayed* are written in SHELX or XYZ formats. The default file names are SHELXxxx.INS and ORTEPxxx.XYZ (where xxx is a number between 001 and 999). Previously files written by ***Ortep-3 for Windows*** will NOT be overwritten. If the originally loaded coordinate file was a SHELX file, then the non-atomic instructions from this file will be copied verbatim to the new file (except for sequence dependent instructions such as AFIX and MOLE which will be removed), otherwise a basic SHELX header is written. The order of atoms follows that in the ATOMS array of ORTEP-III, and will usually be different from that input. Up to the maximum number of 1999 atoms may be listed. This option is useful if the atomic parameters for some portion of the structure (or a set of symmetry equivalent atoms) are desired, or in conjunction with the **Rename Atoms** option.

5.1.6 Write Raster3D File

The atomic contents of the screen *as currently displayed and in the current orientation* are written to the file RASTER3D.DAT, which is a pseudo-PDB type file suitable for input to the Raster3D suite of programs, *e.g.* RASTEP (themal ellipsoid plots), BALLS (van der Waals surfaces) or RODS (rod representation). All these programs write a scene description file which is rendered with the Raster3D program RENDER. The Raster3D suite of programs for UNIX systems may be obtained from the web-site :

http://www.bmsc.washington.edu/raster3d/html/raster3d.html

A Windows version of these programs has been implemented in the WinGX suite of programs available from the web-site :

http://www.chem.gla.ac.uk/~louis/software/wingx/

5.1.7 Write POV-Ray File

The contents of the screen *as currently displayed and in the current orientation* are written to a POV-Ray scene description file ORTEPxxx.POV. The colour information about atoms, background, lettering *etc* is also passed to this file, so that a ray traced picture corresponding to the exact current screen illustration may be obtained. There is a choice as to the representation of atoms in the POV-Ray picture, as either standard ORTEP type thermal ellipsoids, as RMSD or MSD (PEANUT type) surfaces, as ball-and-stick models, as van der Waals surfaces or as rod representation. This file is rendered by the freely available ray-tracing program POV-Ray, which is obtainable as an executable for a number of different platforms from the web-site

http://www.povray.org

Version 3.1 of POV-Ray (the current version) is required for the files written by this program. ***Ortep-3 for Windows*** has a GUI which allows some customisation of the view, but the scene description language of POV-Ray is highly complex and flexible. Manual editing of the file written by ***Ortep-3 for Windows*** will often be necessary to obtain a desired final graphic. Some care has been taken to make the scene description file easy to modify. Most of the variables (apart from the individual atomic positional parameters, quadric coefficients used to describe the thermal ellipsoids and coordinates of bonds) are declared in the header at the top of the file and need only be modified in this one place. Each bond is recalculated from the interatomic distances when the POV-Ray file is written, so that excluded bonds will re-appear

in the POV-Ray picture. Since each bond is clearly annotated in the file, it is a relatively easy matter to delete unwanted bonds. An example of such a header is shown below :

```
#include "colors.inc"
#include "textures.inc"
#include "metals.inc"
#declare Bond_Texture     = texture {
                            pigment {color Black }
                            finish { Metal } }
#declare HBond_Texture    = texture {
                            pigment {color Black }
                            finish { Metal } }
#declare Texture_C        = texture {
                            pigment {color SkyBlue }
                            finish { Shiny } }
#declare Texture_H        = texture {
                            pigment {color Green }
                            finish { Shiny } }
#declare Texture_N        = texture {
                            pigment {color BrightGold }
                            finish { Shiny } }
#declare Texture_O        = texture {
                            pigment {color Firebrick }
                            finish { Shiny } }
#declare H_Radius         = 0.05;
#declare HBond_Radius     = 0.02;
#declare Bond_Radius      = 0.02;
#declare    Radius_C      = 0.77;
#declare    Radius_H      = 0.32;
#declare    Radius_N      = 0.70;
#declare    Radius_O      = 0.66;
#declare    Radius_Scale  = 0.33;
#declare Bond_Truncate    = 0;
#declare View_Distance    = 36.5;

global_settings { assumed_gamma 2.2 ambient_light rgb < 1, 1, 1 > }
camera {
        location < 0.0 , 0.0 , View_Distance >
        angle     20.0
        up       < 0.0 , 1.0 , 0.0 >
        right    <-1.33, 0.0 , 0.0 >
        look_at  < 0.0 , 0.0 , 0.0 >
       }
background { color SteelBlue }
light_source { < 0.0,   0.0, 100.0 >
      color red 2.0 green 2.0 blue 2.0 }
```

The textures (*i.e.* colours and finishes) of each atomic type and the standard bonds and bonds to H atoms may be modified by editing each entry

```
#declare Texture_C        = texture {
                            pigment {color SkyBlue }
                            finish { Shiny } }
```

Note that case is important in all declarations, *e.g.* SkyBlue is not the same as skyblue. In this example a ball and stick representation is being described and the radius of atomic types (in Å) and the bonds may be set individually and the overall scale set by:

```
#declare    Radius_N      = 0.70;
#declare    Radius_O      = 0.66;
#declare    Radius_Scale  = 0.33;
```

ORTEP style thermal ellipsoids may be drawn as plain ellipsoids, ellipsoids with the boundary ellipses or cutout ellipsoids. Bonds are normally drawn from atomic centre to atomic centre. Since the ellipsoids or other atomic representations are solid objects in the POV-Ray world this is normally invisible, but in the case of cutout ellipses this may become visible. There is an option to truncate all bonds to cutout ellipses at the ellipse surface (which is how ORTEP-III draws bonds) but as this increases the rendering time by a factor of 3-5 it is available as an option. The easiset way to use this facility is to deselect Truncate bond in the POV-Ray Interface GUI (actually you need do nothing since this is the default) and when the required illustration is ready a final rendering can be made with this option set on by modifying the scene description file and declaring the variable Bond_Truncate to have any value other than zero. *e.g.*

```
#declare Bond_Truncate    = 1;
```

The view distance is set automatically but is not always correct. To zoom in, declare View_Distance with a smaller value, to zoom out, with a larger value.

```
#declare View_Distance    = 36.5;
```

The global settings will not normally need adjustment, but the user is encouraged to read the (unfortunately very extensive) POV-Ray documentation to find out more about the POV-Ray scene description language.

5.1.8 Exit ORTEP3

Quit **Ortep3 for Windows** program. No confirmatory prompt is given.

5.2. CONTENTS MENU

The items from this menu control the contents of the illustration, *i.e.* those atoms to be drawn. By default, and for all new coordinate data sets read in, the **Use Asymmetric Unit** mode will be made active. The menu items **Use Asymmetric Unit, Grow Fragment** and **Unit Cell Contents** are ganged, so that only one may be active.

5.2.1 Use Asymmetric Unit

If this option is active, the entire asymmetric unit forms the contents of the illustration, unless some atoms have been specifically excluded by other options (see **5.2.6 - 5.2.11**). This mode is the default mode for displaying a new structure.

5.2.2 Grow Fragment

If this mode is active, a symmetry expansion of incomplete fragments which are situated about crystallographic symmetry elements is performed The **auto-mode** is generally most effective; all atoms in the input file are treated as seed atoms, which results in the symmetry expansion of ALL the incomplete fragments in the asymmetric unit. Alternatively, the user can select **User-define** which will prompt for a specific seed atom and search radius. This will result in the symmetry expansion of the fragment containing this seed atom, with other

non-connected fragments being ignored. If the structure is polymeric, then this process will continue until the atoms array is filled (this may take a while to complete, as 1999 atoms can now be drawn !!)

5.2.3 Unit Cell Contents

This menu item draws the unit cell contents. The **auto-mode** will result in an illustration with the entire contents of one unit cell, and where all molecules which have at least one atom within the unit cell are completed. If the structure is polymeric, then this process will continue until the atoms array is filled. The **user-define** mode allows the user to specify how many unit cells in all three directions are required. These will be centred about the midpoint of the primary unit cell. In this mode it is also possible to choose whether all molecules are completed, and whether the cell outline is drawn. The default action is identical to **auto-mode**. Selecting the **Unit Cell Contents** option will automatically switch off all labels.

5.2.4 Sphere of Enclosure

All atoms within a sphere of user defined radius, about a user defined atom, are included in the illustration. This option does NOT expand all fragments, and hence allows the drawing of polymeric or infinite lattice structures.

5.2.5 Box of Enclosure

All atoms within a Cartesian box of user defined dimensions, about a user defined atom, are included in the illustration. This option does NOT expand all fragments, and hence allows the drawing of polymeric or infinite lattice structures. If the user wishes to have an enclosure box based on the unit cell vectors for such structures, then the **Unit Cell Contents** item **Auto Mode** should be selected, *and the Expand all fragments option must be switched off*.

5.2.6 ADR Add/Subtract/Reset

This item allows the user to specically include or exclude or remove an atom designator run (ADR) so that a specified part of the unit cell, for example, may be drawn. The user is referred to the ORTEP-III manual for a detailed explanation of the term ADR.

5.2.7 Include H Atoms

This item and the next one form a toggle. If active (this is the default condition), H atoms will be drawn with the appropriate graphic representation (see the **Thermal-H** menu item, page 20).

5.2.8 Exclude H Atoms

If this control is active, no H atoms will be drawn. The view orientation might change slightly if the default view option (**Best View** see **5.5.1**) is active.

5.2.9 Exclude Options

This menu item allows the user to exclude atoms from the illustration by a variety of ways.

5.2.9.1 Element Type	Exclude all atoms of specified elemental type(s)
5.2.9.2 Named Atoms	Exclude all atoms with specified name, including all its symmetry equivalents

5.2.9.3 Selected Atoms Exclude all atoms selected by mouse clicks. The symmetry equivalents are NOT excluded by this option.

5.2.9.4 Atoms+SYMM Identical to above, except that symmetry equivalents WILL be excluded.

5.2.10 Restore Options

This menu item allows the user to restore atoms which have been excluded by any of the above operations

5.2.10.1 Element Type `Restores all atoms of specified elemental type(s),*except* those selected by item **5.2.9.3** above.

5.2.10.2 Named Atoms Restores all atoms with specified name, including all symmetry equivalents.

5.2.10.3 Selected Atoms Restores all atoms selected by mouse clicks (*i.e.* items **5.2.9.3** and **5.2.9.4** above.)

5.2.10.4 All Non-H atoms Restore all atoms.

5.2.11 Select by Part No.

This menu item allows a user to select part of the structure using the SHELXL PART instructions. It is only available if the loaded file is a SHELX file and if that file contains PART instructructions (otherwise this control is greyed). This is most useful when the structure contains extensive disordered sections where it is desired to show only one component of the disorder.

5.2.12 Add Centroid

This menu item initiates a mouse driven routine to select atoms for a centroid calculation. Up to 200 atoms may selected in this way. The resultant centroid is included in the atoms list with a label Ctxx (xx ranging from 01 to 99) and a covalent radius of 0.77Å (the same as a C-atom). A maximum of 100 centroids may be added in this way. Centroids generated in this way will not be drawn, but all bonds from these pseudo-atoms to all others which are longer than the parameter **CentroidBondMin** will be drawn as dashed lines. The value of the parameter **CentroidBondMin** may be modified using the **Change Ortep Parameters** menu item This routine is particularly useful for drawing bonds from transition metals to π-bonded ring systems.

5.2.13 Invert Model

The chirality of the model is switched by inversion through the origin. This will produce the alternate enantiomer of the asymmetric unit, but if the space group is one of the 11 pairs of enantiomeric space groups, or one of the following *F*dd2, $I4_1$, $I4_122$, $I4_1md$, $I4_1cd$, *I*-42d or $F4_132$, then the translational components will be incorrect for packing diagrams (see Bernardinelli & Flack, *Acta Cryt* (1985) **A41**, 500-511).

5.2.14 Display Crystal Data

Crystallographic information stored for ORTEP is displayed in a message box.

5.3. STYLE MENU

This menu controls the stylistic features of ORTEP, *i.e.* the exact graphical representation of the atomic thermal ellipsoids and interatomic bonds.

5.3.1 Select New Style

Four stylistic templates are available in **Ortep3 for Windows**, called somewhat arbitrarily **Organic**, **Inorganic**, **Organometallic** and **PLUTO**. These provide the basis for the graphical representations of ORTEP. The **PLUTO** style draws each atomic type as a sphere, with a radius proportional to the covalent radius. The other styles draw each atom as a thermal ellipsoid (save for hydrogen atoms) in various forms. The **Stick** mode is useful to get a suitable view quickly, as it is drawn much more rapidly. In this mode, bonds are drawn as simple lines, and atoms are represented by an asterix.

Thermal-H is not a style but an option. For all the styles mentioned above, hydrogen atoms will be drawn as spheres (by default 0.1 Å), with thin bonds. If the user wishes to draw hydrogen atoms with their refined thermal parameters (usually isotropic, but possibly anisotropic for neutron-diffraction structural analyses), then the **Thermal-H** option should be selected. All bonds to H-atoms will then be of the "standard" type (see **4.2** and **5.3.7**)

5.3.2 Change ORTEP Parameters

As mentioned above, many of the parameters controlling the GUI and the operation of ORTEP may be modified dynamically through this menu item. A parameter box will be displayed when this menu item is selected, and any number of parameters may be modified. The program will not accept unsuitable values. The most common parameters which the user may wish to modify **EllipsoidProbability**, **ScreenLine-Width** and **StereoDisplacement** may also be modified using the **ORTEP-3 Quick Menu**. This is obtained by a *right mouse-button click* anywhere on the graphics screen. A number of preset values are obtainable. The meaning of all the parameters are given in Table 1 below.

5.3.3 Reset to Default Style

This menu item resets the style to the default for the currently selected style. This will only have an effect if the graphical representation of elements, atoms or bonds have been changed using **Set Element Style**, **Selected Atom Style**, **Set Bond Style**, **Selected Bond Style**. This option will also restore any deselected bonds.

5.3.4 Set Element Style

This item allows the user to change globally both the *graphical representation* of a particular element, and the value of the stored *covalent radius*. In practise, adjustment of the NPLANE, NDOT, NLINE and NDASH parameters for the Custom Ellipsoid Style allows an element to be represented by any of the ellipsoid components available in ORTEP-III (see Fig 1). A self-explanatory dialog box is presented for modifying the ellipsoid representation. The default

colours for all atomic types (the CPK colour scheme) are defined in the file ATOMCOLS.DEF. The user may ascribe any colour to any atom.

5.3.5 Selected Atom Style

It is also possible to draw any *individual* atom or sets of atoms in a selected style different from the standard element style set by **Set Element Style**. Selected styles are possible for up to 20 different individual atom or sets of atoms. A self-explanatory dialog box is presented for modifying the ellipsoid representation.

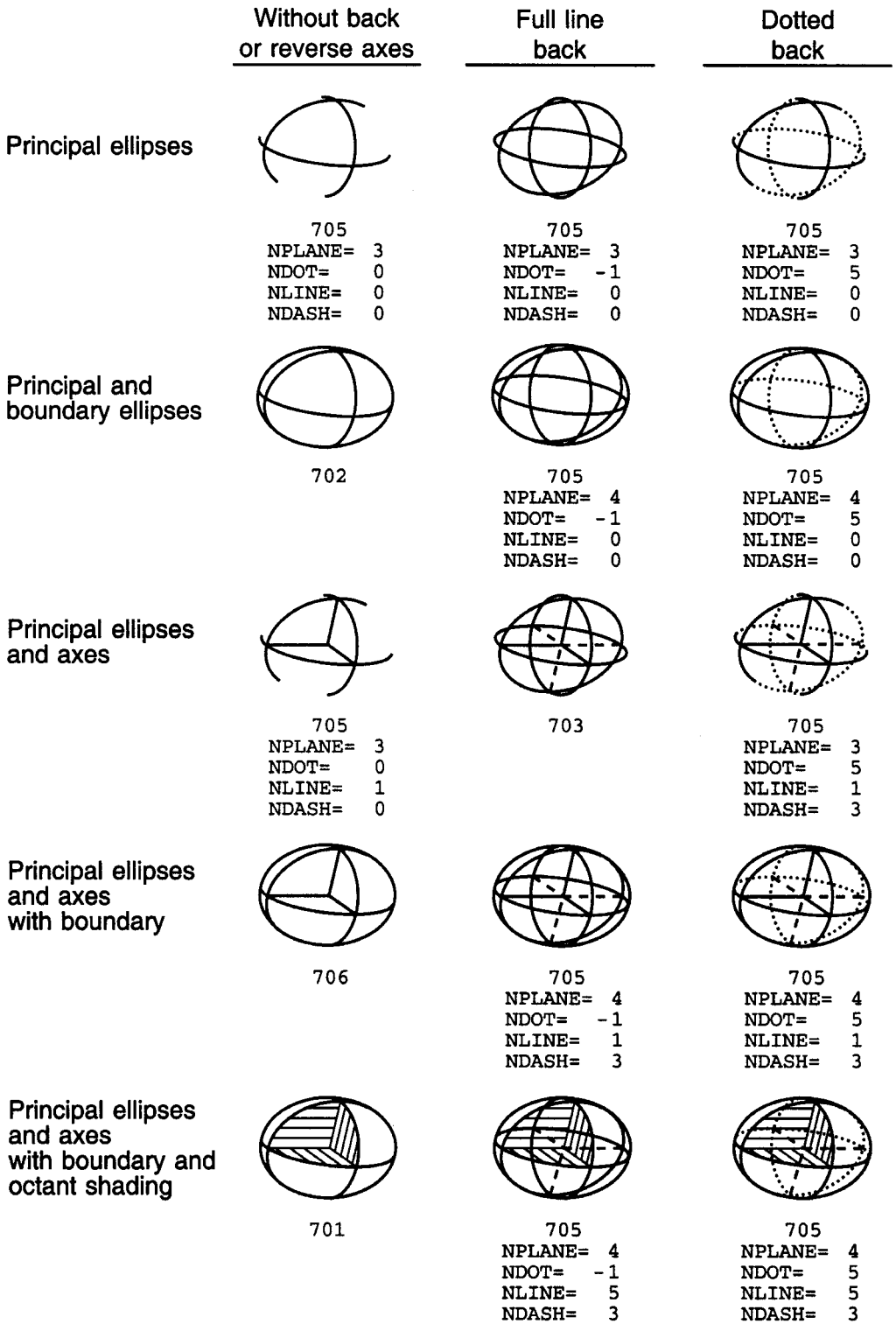

Fig 1. Various combinations of ellipsoid components showing ORTEP instruction number and parameter values to produce each.

5.3.6 Draw No Atoms

If active this menu item bypasses the drawing of all atoms, but leaves all the bonds in place. It may be useful in certain circumstances.

5.3.7 Set Bond Style

This item allows the user to modify globally the appearance of the standard bond. All the possible bond styles available in ORTEP-III are also available in **Ortep3 for Windows**. Both the number of fill-lines, bond width and bond colour may be modified, and dashed bonds may also be drawn.

5.3.8 Selected Bond Style

This menu item allows the user to select up to 20 bonds or sets of bonds to be drawn in a selected fashion, different from the standard bond style. This option is useful for drawing weak interactions, hydrogen bonds *etc*.

5.3.9 Draw No Bonds

If active this menu item bypasses the drawing of all bonds, but leaves all the atoms in place. It may be useful in certain circumstances, for instance packing diagrams of ionic crystals.

5.3.10 Delete Selected Bond

This menu item initiates a mouse-driven routine allowing the user to select any number of individual bonds to be removed from the illustration. All symmetry equivalent sets of bonds will be removed by this option.

5.3.11 Restore Selected Bond

This menu item initiates a mouse-driven routine allowing the user to restore any number of individual bonds which have been removed by the above option. All symmetry equivalent sets of bonds will be restored by this option. All such restored bonds will be of the “standard” type.

5.3.12 Delete All Bonds

This menu item removes all bonds from the illustration. It differs from **Draw No Bonds** in that bonds may be restored selectively or globally using items **5.3.11** or **5.3.13** respectively.

5.3.13 Restore All Bonds

This menu item will restore ALL bonds deleted with the items **5.3.10** or **5.3.12**. All such restored bonds will be of the “standard” type.

5.3.14 Retrace

If this menu item is active, certain lines will be made heavier than others by retracing over the path several times with a slight displacement. The displacement is set by the ORTEP Parameter **RetraceDisplacement** which is given a suitable default value. **NOTE** that this option results in considerably longer drawing times.

5.3.15 Stereo

If this item is active then a stereo pair of illustrations are drawn. These are rotated relative to each other by the ORTEP parameter **StereoRotationAngle** and the pair of drawing are separated by a distance given by **StereoDisplacementDistance.** The defaults supplied in ***Ortep3 for Windows*** may not be suitable in all cases, and the user should use her/his discretion. The view distance is automatically set to 30 in for stereo plots to give a realistic depth for stereopsis, though the user may modify this value through the ORTEP parameter **StereoViewDistance**. Certain other options are not possible if this mode is active, *e.g.* mouse labelling (since it is very important that the labels have the correct displacement for both drawings). If stereo plots with mouse labels are required, then the mono view should be previously mouse labelled, and the **ORTEP font** will be automatically selected.

5.3.16 Title

If active, this option will draw a title string. The title string is taken from a TITL or TITLE card, but a dialog box is presented so that the user may modify the string as desired. The title will be placed in the bottom left corner of the illustration.

5.4. LABELS MENU

See Section **4.1** concerning the recommendations about atom labelling for ***Ortep-3 for Windows***.

5.4.1 Labelling Mode

Five labelling modes are provided, and these are all ganged so that only one can be active at any time. The automatic placement of labels is implemented through ORTEP-III, but since this option utilises the same *x*-*y* displacement of atom labels from all atomic centres, it is usually unsatisfactory for final output. It may be useful however in recognising atoms in the initial stages of drawing. The *x*-*y* displacement of atom labels is set by the ORTEP parameters **LabelTextXOffset** and **LabelTextYOffset.**

The recommended method of labelling is the **Mouse Labelling** mode. This routine is not part of ORTEP-III and is provided by the GUI. It is only sensible to use this mode once a final satisfactory view has been obtained (subsequent rotations and translations are NOT applied to these mouse labels). The positions of, and the character strings for the labels are set and stored by the menu item **Set Mouse Labels**. If **Mouse Labelling** is selected, and there are no currently stored labels, then the **Set Mouse Labels** routine is automatically called. If stored labels are present, then the illustration will be drawn with these labels. Two types of font, GUI and ORTEP are available (see **4.6**)

5.4.2 Set Mouse Labels

The user should select an atom for labelling, upon which a blue(or red) dot will appear at the atomic centre. The cursor then changes to a cross-hair, and the label position should be selected using left mouse clicks. The left-bottom corner of the label will be placed near the cross-hair position. The intermediate label is also shown in blue (or red), and it is always displayed in the graphics font. If the ORTEP font option has been selected for the final picture, then choose a graphics font size similar to that of the ORTEP font size, to facilitate

accurate placement of labels. A right mouse-button click will confirm the label position, then the cursor changes back to the standard arrow pointer and the colour of the label reverts to the currently selected label colour (white by default). As many atoms as required may be labelled in this fashion. When placing labels using the mouse pointer, remember that as the font-size is increased, the label will "grow" from the left-bottom corner both upwards and in the right direction. If the **Print Graphics Screen** (see **5.6.6**) option is used, true WYSIWYG output is obtained. Unit cells may be labelled in the same way as atoms (the corners of the unit cells are pseudo-atoms).

If two or more symmetry equivalent atoms are present in the illustration, the labels for these atoms are automatically adjusted to indicate the ORTEP symmetry operation number(s). An extra trailing underscore '_' (see **5.4.4**) followed by up to six symmetry indicator characters is added (inside any brackets if present) to the label, for all symmetry positions except the primary position (equivalent position #1) of the asymmetric unit. These symmetry indicator characters are by default the numbers 2 - 96, though they may be changed if desired (see **Symmop Symbols 5.4.6**).

5.4.3 Delete Mouse Labels

This option allow the user to delete all mouse labels or individual labels which have been added by accident.

5.4.4 Underscore on Labels

If this option is active, an underscore will be placed between the label and the symmetry indicator characters. For atoms in equivalent position #1, no symmetry indicator characters are added. If this control is NOT active and the **Mouse Labels (GUI Font**) is selected, then the PostScript and HPGL files will have the symmetry indicator characters for the mouse labels drawn as *superscripts*, thereby complying with *Acta Cryst* requirements for symmetry designators in the labels.

5.4.5 Brackets on Labels

If this option is active, brackets will be drawn around the numerical part of the atom label.

5.4.6 Symmop Symbols

This menu item allows the user to change dynamically the default character set for the label-symbols corresponding to the ORTEP symmetry operator numbers (see **5.4.2**). These numbers are the final two digits in the atom designator code (see ORTEP-III manual); the corresponding symmetry operators may be listed using the menu item **List Symmops** in the **CALCULATE** menu (see **5.8.3**). The default symbols are the integer characters ' 2' - '96'. A parameter box is displayed, and any number of these symbols may be modified. It is also possible to modify this character set by using the ORTEP3.INI file (see page 9). This latter method is more useful if the user normally requires an alternative character set. If the symbol for any particular symmetry operation number(s) is set to a blank, then no extra characters are attached to the atom labels.

5.5. VIEW MENU

This menu consists of several viewing-modes which are all ganged, so that only one may be active at any time. The default, and usually the most satisfactory starting view is **Best View**. When any of these modes are selected, all stored rotations and translations are set to zero.

5.5.1 Best View

This option calculates the mean plane, and sets the highest axis of inertia of the molecule normal to the screen. This will usually give the view with the least overlap, *i.e.* the 'best view'. Occasionally (*e.g.* if the molecule comprising the illustration has perfect spherical symmetry such as a tetrahedron or octahedron) it is not possible to calculate a 'best view'. The program then issues a warning message on the status bar, and prompts the user to select another view-mode.

5.5.2 Standard View

This option places the centroid of the molecule in the centre of the screen, with the crystallographic ***a*** axis vertical, and the $\boldsymbol{c}^*$ axis normal to the screen.

5.5.3 Select Normal Plane

This option allows the user to select three atoms by mouse clicks, which form a plane. The three atoms should be non-colinear, but the algorithm is quite robust, and virtually colinear atoms may be chosen without a program error. The view direction is then set normal to this plane, with the screen X-direction set along the vector atom1-atom2 and with the vector atom1-atom3 lying in the screen XY-plane in the +ve Y direction (upwards).

5.5.4 Select Edge Plane

This option is identical to the above, except that the view direction is set to be along the chosen plane, so that the viewer sees this plane edge-on.

5.5.5 View Normal To (100) { (010), (110) }

These options provide views where the crystallographic ***bc***, ***ac***, ***ab*** planes respectively are placed in the plane of the illustration. The first axis of the pair lies along the screen *x*-direction (horizontal), with the second axis lying in the *xy*-plane (*i.e.* plane of the screen). The $\boldsymbol{a}^*$ axis *etc* is normal to the screen, and for crystal systems with orthogonal axes (orthorhombic, tetragonal, cubic), these views correspond to views down the crystallographic ***a***, ***b*** and ***c*** axes respectively.

5.5.6 Continuous Rotation

This option allows continuous rotation of the illustration through the current rotation angle. The default direction if +X, but this direction may be changed by hitting the following keys:

Arrow up	-X
Arrow down	+X
Arrow left	-Y
Arrow right	+Y

Page up +Z

Page down -Z

The rotation may be halted by hitting any other key (apart from some control keys) or by depressing the mouse button in the graphics area for several seconds.

5.6. GRAPHICS MENU

This set of menu options control how the illustration appears on the graphics screen, and also the production of hardcopy and metafile output from the screen graphics

5.6.1 Select Colour

The colours assigned to all graphical objects - atoms types , bonds, text (labels and title), unit cell outline, foreground (used only for monochrome illustrations) and background may be modified from this menu item. Any loaded colour may be chosen without restriction for each graphical object.

5.6.2 Background Style [Plain/Graduated/Patterned]

The background may be drawn as a plain colour, graduated from black at the top of the screen to the selected colour at the bottom or patterned. Note that the graduated or patterned backgrounds use many colours and are only effective for colour depths of 16-bit colour or greater. They look odd on a 256-colour display and quite ridiculous on a 16-colour display. The **Patterned** option uses a 2-dimensional Fourier series to produce variations in the colour intensity (similar to that used in SCHAKAL). The ORTEP Parameter **PatternNumber** controls the number of terms used in the Fourier summation (and changes the pattern). The patterned background takes some time to calculate, but is stored and only recalculated if the background colour or **PatternNumber** are changed.

5.6.3 Colour Plot/Monochrome Plot

The user may select either a monochrome, or a colour illustration. The latter is the default, but the former is recommended if the **Print Graphics Screen** option is to be used with an attached printer which does not support colour. The monochrome mode uses the foreground colour (default White) selected in **5.6.1** above.

5.6.4 Clear Graphics Screen

This option clears any illustration from the graphics screen.

5.6.5 Select Graphics Font

The Graphics Font (point size, colour, effects and font style) used for the labels and title-text may be selected from a dialog box. Any loaded Windows font may be chosen, though clearly some are much more suitable than others. Only those labels set by the mouse labelling routine will use this font. These labels may also be used for the metafile outputs (see **5.1.4**) The HPGL format has only one font-type (pseudo Courier) but there are more fonts available in PostScript output. The program will choose the closest PostScript font to the current Graphics Font.

5.6.6 Print Graphics Screen

With this option, the current illustration is copied directly to an attached printer. This facility uses the Microsoft printer drivers, so the actual result will depend on local conditions. It has not been tested on a large number of printers, but the copy obtained from HP laser printers is of excellent quality. There are two choices for the print size - landscape A4 or direct journal size (DJS). Many primary journals *e.g.* ACS journals now ask for illustrations at the correct size for direct reproduction. The sizes of the A4 plot is handled automatically - the height will be the maximum resolution of your printer and the width chosen to retain the horizontal/vertical aspect ratio of 4:3. The size of the DJS plot is now handled by the ORTEP parameter **DJS_ScalingFactor** which is the proportion relative to the landscape A4 plot (default 0.25). The linewidths for each format are chosen automatically and will depend on the **PlotLineWidth** used for the screen display (normally 1). It is possible to tweak the plotted linedwidth using the ORTEP Parameters **PlotA4_LWScale** and **PlotDJS_LWScale** which are normally set to 1.0. The user may need to experiment to get suitable settings of these parameters. Instead of printing the illustration directly, is also possible to save the plot as a plot-file (from the Printer Dialog Box). The format of this plot-file will depend on the local printer, *e.g.* for a LaserJet 4ML, it is in PostScript (Microsoft dialect).

5.6.7 Copy To Clipboard

This menu item copies the current illustration *exactly as is* to the clipboard. This may subsequently be inserted into another Windows program *e.g.* a word-processor or graphics processor program.

5.6.8 Export as BMP file

The screen illustration may also be saved as a metafile in the Windows BMP format. The file will be called ORTEPxxx.BMP and previous versions will not be overwritten.

5.6.9 Draw Frame

By default a frame is drawn around each illustration. Deselecting this item will remove the frame. The ORTEP Parameter **DrawFrame** should be set to “no” in the ORTEP3.INI file if you wish the default to be no frame.

5.7. OPTIONS MENU

These menu items allow the user to make rarely required changes to the standard settings.

5.7.1 Immediate Graphics

Normally the final picture is only displayed when the graphics calculations are complete. For some complicated illustrations, this may take several seconds, resulting in a disconcertingly long wait. If this item is active, the illustration will be drawn as it is calculated. **NOTE** however that this will result in substantially longer drawing times.

5.7.2 Overlap Correction

If this item is active, the overlap between atoms and bonds will be calculated. This is the default. The actual margin left around overlapped atoms can be modified through the ORTEP parameter **OverlapMargin**.

5.7.3 Rename Atoms

This option allows the user to rename atoms by mouse-selection. The new label MUST conform to the suggested atomic naming scheme (see **4.1**)

5.7.4 POV-Ray/PostScript Viewer/HPGL Viewer

This option allows the user to launch POV-Ray from within ***Ortep-3 for Windows*** using the last created POV-Ray scene description file as input. The ORTEP Parameter **POVRayExecutable** needs to be set in the ORTEP3.INI file to the fullpath name of the POV-Ray executable on your system. Similarly the PostScript and HPGL files written may be examined with viewer programs (see page 32 for sources of such programs).

5.8. CALCULATE MENU

These menu items show the results of geometrical calculations, RMS analysis of the anisotropic thermal parameters, or display some current parameters.

5.8.1 List Bonds, List Angles, List RMS

Either all bonds, all angles or all RMS displacements of the adp's are calculated by ORTEP-III, and the raw list output is shown in a scrollable box.

5.8.2 List Atoms

All atoms in the illustration are listed with their names, symmop numbers and unit cell translations.

5.8.3 List Symmops

The current ORTEP symmetry operators are shown with their number, so that symmops may be related to the graphic symbols used for the labels (see **5.4.2** and **Symmop Symbols 5.4.6**).

5.8.4 Interactive GEOM

With this menu item, either 2, 3 or 4 atoms may be mouse-selected for bond distance, bond angle or torsion angle calculations. If two atoms A,B are selected, the A-B distance in Å is displayed. If three atoms A,B,C are selected, the angle A-B-C is displayed, together with the A-B and B-C distances in parentheses. If four atoms A,B,C,D are selected, the torsion angle A-B-C-D is displayed, together with the A-B, B-C, C-D distances and the A-B-C and B-C-D angles in parentheses. If more than 4 atoms are selected, or if the OK button (or right mouse-button) is clicked, the selection array is cleared for another calculation.

Table 1 ORTEP Parameters

ORTEP Parameter	Meaning	Default value
BondSearchDistanceMax	Maximum allowable bond distance (Å)	4.0
BondSearchDistanceMin	Minimum allowable bond distance (Å)	0.65
BondToleranceFactor	The maximum searchable bond distance between two atoms A and B is the sum of their covalent radii plus this parameter (Å)	0.2
CentroidBondMin	Minimum bond distance (Å) for added centroids	1.65
DJS_ScalingFactor	Proportion of direct journal size (DJS) plot relative to Landscape A4 plot.	0.25
EllipseSmoothingParameter	Smaller values produce a smoother ellipsoid. Allowed values in the range 0.0 - 3.0	1.0
EllipseProbability	Percentage probability for thermal ellipsoids; range 10-99	50
LabelTextXOffset	Horizontal offset for label placement (in)	0.45
LabelTextYOffset	Vertical offset for label placement (in)	0.45
MessageDelay	Time (in secs) for display of error messages on the status bar	2.0
OverlapMargin	Margin around overlapped bonds and atoms	0.04
PatternNumber	Number of terms in Fourier summation for patterned background (1-20)	20
PerspectiveViewDistance	Perspective view distance for standard plots	30.0
PlotA4_LWScale	Linewidth scaling factor for **Print Graphic Screen** hardcopy output (A4)	1.0
PlotDJS_LWScale	Linewidth scaling factor for **Print Graphic Screen** hardcopy output (DJS)	1.0
PlotLineWidth	Linewidth factor for all plots (arbitary unit)	1
PlotMargin	Blank margin around drawing (in)	0.1
PlotScaleFactor	Scale factor for non-automatic scaling	0.9
RetraceDisplacement	Displacement for retracing lines (in)	0.005
StereoDisplacement	Distance between the two images in a stereo plot (in)	4.0
StereoRotationAngle	Rotation angle (+ and -) for stereo plots (deg)	2.7
StereoViewDistance	Perspective view distance for stereo plots	30.0
StereoViewScaleFactor	Scale factor used for stereo plots	0.32
SupescriptDisplacement	Vertical displacement of superscript text in proportion of font size	0.5
SuperscriptSize	Size of superscript text in proportion of font size	0.8
UnitCellAxisLabel_A(B/C)	Label for the A (B/C) unit cell corner	A (B/C)
UnitCellOrginLabel	Label for the unit cell origin	ORGN
AutoFileNaming	If “no” prompts for saved filename	yes (/no)
FontName	Font to be used for all windows	Arial
FontPointSize	Point size of windows font	10
GraphicsFontName	Font to be used for labels/text	Arial
GraphicsFontPointSize	Point size of labels/text font	14
HyperTextChars	Number of characters in hypertext help per line	70
HyperTextLines	Number of lines in hypertext window	24
InitialPlotStyle	Determines whether colour or monochrome display	colour (/mono)
StatusBarPosition	Poistion of status bar above or below graphics window	bottom (/top)
DrawFrame	Whether frame is drawn as default	yes (/no)
POVRayExecutable	Fullpath name of POV-Ray executable	no default
PostScriptExecutable	Fullpath name of PostScript interpretor (eg GSview)	no default
HPGLExecutable	Fullpath name of HPGL interpretor (eg PRINTGL)	no default
BackGroundColor	Default colour of background	Black
ForeGroundColor	Default colour of foreground (monochrome plots)	White
UnitCellOutline	Default colour of unit cell edges	Yellow
BondColor	Colour of standard bonds	White
TextColor	Default colour of labels and title font	White
POVRayFloorColor	Default floor colour for POV-Ray	DkGreenCopper
POVRayCutoutColor	Default cutout colour for POV-Ray ellipsoids	RichBlue
POVRayEquatorColor	Default equator colour for POV-Ray ellipsoids	Black

Table 2. Colour names and RGB values defined in *Ortep-3 for Windows*

Colourname	R	G	B	Colourname	R	G	B
Aquamarine	0.439216	0.858824	0.576471	IndianRed	0.309804	0.184314	0.184314
BakersChoc	0.36	0.2	0.09	Khaki	0.623529	0.623529	0.372549
Black	0	0	0	LightBlue	0.74902	0.847059	0.847059
Blue	0	0	1	LightGray	0.658824	0.658824	0.658824
BlueViolet	0.62352	0.372549	0.623529	LightGrey	0.658824	0.658824	0.658824
Brass	0.71	0.65	0.26	LightSteelBlue	0.560784	0.560784	0.737255
BrightGold	0.85	0.85	0.1	LightWood	0.91	0.76	0.65
Bronze	0.55	0.47	0.14	LimeGreen	0.196078	0.8	0.196078
Bronze2	0.65	0.49	0.24	Magenta	1	0	1
Brown	0.647059	0.164706	0.164706	MandarinOrange	0.89	0.47	0.2
CadetBlue	0.372549	0.623529	0.623529	Maroon	0.556863	0.137255	0.419608
Clear	1	1	1	MediumAquamarine	0.196078	0.8	0.6
CoolCopper	0.85	0.53	0.1	MediumBlue	0.196078	0.196078	0.8
Copper	0.72	0.45	0.2	MediumForestGreen	0.419608	0.556863	0.137255
Coral	1	0.498039	0	MediumGoldenrod	0.917647	0.917647	0.678431
CornflowerBlue	0.258824	0.258824	0.435294	MediumOrchid	0.576471	0.439216	0.858824
Cyan	0	1	1	MediumSeaGreen	0.258824	0.435294	0.258824
DarkBrown	0.36	0.25	0.2	MediumSlateBlue	0.498039	1	
DarkGreen	0.184314	0.309804	0.184314	MediumSpringGreen	0.498039	1	
DarkOliveGreen	0.309804	0.309804	0.184314	MediumTurquoise	0.439216	0.858824	0.858824
DarkOrchid	0.6	0.196078	0.8	MediumVioletRed	0.858824	0.439216	0.576471
DarkPurple	0.53	0.12	0.47	MediumWood	0.65	0.5	0.39
DarkSlateBlue	0.419608	0.137255	0.556863	Mica	0	0	0
DarkSlateGray	0.184314	0.309804	0.309804	MidnightBlue	0.184314	0.184314	0.309804
DarkSlateGrey	0.184314	0.309804	0.309804	Navy	0.137255	0.137255	0.556863
DarkTan	0.59	0.41	0.31	NavyBlue	0.137255	0.137255	0.556863
DarkTurquoise	0.439216	0.576471	0.858824	NeonBlue	0.3	0.3	1
DarkWood	0.52	0.37	0.26	NeonPink	1	0.43	0.78
DimGray	0.329412	0.329412	0.329412	NewMidnightBlue	0	0	0.61
DimGrey	0.329412	0.329412	0.329412	NewTan	0.92	0.78	0.62
DkGreenCopper	0.29	0.46	0.43	OldGold	0.81	0.71	0.23
DustyRose	0.52	0.39	0.39	Orange	1	0.5	0
Feldspar	0.82	0.57	0.46	OrangeRed	1	0.498039	0
Firebrick	0.556863	0.137255	0.137255	Orchid	0.858824	0.439216	0.858824
Flesh	0.96	0.8	0.69	PaleGreen	0.560784	0.737255	0.560784
ForestGreen	0.137255	0.556863	0.137255	Pink	0.737255	0.560784	0.560784
Gold	0.8	0.498039	0.196078	Plum	0.917647	0.678431	0.917647
Goldenrod	0.858824	0.858824	0.439216	Quartz	0.85	0.85	0.95
Gray	0.752941	0.752941	0.752941	Red	1	0	0
Gray05	0.05	0.05	0.05	RichBlue	0.35	0.35	0.67
Gray10	0.1	0.1	0.1	Salmon	0.435294	0.258824	0.258824
Gray15	0.15	0.15	0.15	Scarlet	0.55	0.09	0.09
Gray20	0.2	0.2	0.2	SeaGreen	0.137255	0.556863	0.419608
Gray25	0.25	0.25	0.25	SemiSweetChoc	0.42	0.26	0.15
Gray30	0.3	0.3	0.3	Sienna	0.556863	0.419608	0.137255
Gray35	0.35	0.35	0.35	Silver	0.9	0.91	0.98
Gray40	0.4	0.4	0.4	SkyBlue	0.196078	0.6	0.8
Gray45	0.45	0.45	0.45	SlateBlue	0	0.498039	1
Gray50	0.5	0.5	0.5	SpicyPink	1	0.11	0.68
Gray55	0.55	0.55	0.55	SpringGreen	0	1	0.498039
Gray60	0.6	0.6	0.6	SteelBlue	0.137255	0.419608	0.556863
Gray65	0.65	0.65	0.65	SummerSky	0.22	0.69	0.87
Gray70	0.7	0.7	0.7	Tan	0.858824	0.576471	0.439216
Gray75	0.75	0.75	0.75	Thistle	0.847059	0.74902	0.847059
Gray80	0.8	0.8	0.8	Turquoise	0.678431	0.917647	0.917647
Gray85	0.85	0.85	0.85	VeryDarkBrown	0.35	0.16	0.14
Gray90	0.9	0.9	0.9	Violet	0.309804	0.184314	0.309804
Gray95	0.95	0.95	0.95	VioletRed	0.8	0.196078	0.6
Green	0	1	0	VLightGrey	0.8	0.8	0.8
GreenCopper	0.32	0.49	0.46	Wheat	0.847059	0.847059	0.74902
GreenYellow	0.576471	0.858824	0.439216	White	1	1	1
Grey	0.752941	0.752941	0.752941	Yellow	1	1	0
HuntersGreen	0.13	0.37	0.31	YellowGreen	0.6	0.8	0.196078

PRINTING HPGL AND POSTSCRIPT FILES:

Excellent shareware programs are available for printing HPGL and PostScript files on a wide variety of printers. These are available at the following web-sites:

For HPGL files, program PRINTGL is available from the web-site

http://www.concentric.net/~ravitz/

For HPGL files, program SPLOT is available (for small fee) from the web-site

http://www.swplot.com

For PostScript files, program GSVIEW is available from the web-site

http://www.cs.wisc.edu/~ghost/index.html