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DRAWxtl, an open-source computer program to produce crystal structure drawings

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The computer program *DRAWxtl* produces crystal structure drawings in the form of an interactive screen representation, as well as VRML files for use on web pages and in classroom teaching, and creates input files for the popular *Persistence of Vision Raytracer (POV-Ray)* rendering program for publication-quality graphics, including generation of stereo pairs. *DRAWxtl* output produces the standard kinds of graphical representations: spheres, ellipsoids, bonds and polyhedra of any complexity. In addition, it can draw arrows to represent magnetic moments, show capped cones to indicate the location of lone-pair electrons and display Fourier contours in three dimensions. A unique feature of this program is the ability to plot incommensurately modulated and composite structures. This open-source program can be used with operating systems as diverse as Windows (9X, NT, 2000 and XP), Mac OS X, Linux and most other varieties of Unix.

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1. Introduction

The first widely distributed computer program for preparation of crystal structure drawings was *ORTEP* (Johnson, 1964). Although the fixed format input of this program was difficult to use, and the batched computer operations of that era led to long turn-around time between iterations, it was a major advance because of its ability to draw publication-quality graphics with features such as stereo pairs, displacement ellipsoids and later removal of hidden lines. A later major advance was costly specialized computer hardware and software that produced views that could be rotated in real time, greatly enhancing comprehension of the three-dimensional relationships within the structure. As computer hardware and software have improved in quality and speed, these capabilities have become accessible with programs utilizing inexpensive and widely available computers. *DRAWxtl* represents such software.

The program was started by Larry W. Finger (hereafter referred to as LWF) as a plug-in module, written in C, for a specialized graphics system. This module produced no graphics, just files that could be viewed within the display module of the system; however, many of the basic crystallographic operations were coded for that application. That code was adapted by Martin Kroeker to prepare files in the formats required by the Virtual Reality Modeling Language (VRML) and the *Persistence of Vision Raytracer (POV-Ray)* program (Persistence of Vision Pty. Ltd., 2004). VRML is compact and integrated with Internet browsers, allowing crystal structure representations to be viewed embedded within web content. The *POV-Ray* program creates very high quality graphics using ray-traced renderings and complex lighting models. While on leave, LWF had a need to generate structure drawings, which started the collaboration that has resulted in the current version, which also incorporates real-time views of the structure using the OpenGL screen graphics.

The initial versions of *DRAWxtl* only had a command-line interface, partly because a convenient and portable open-source graphical

user interface (GUI) toolkit was not available. Restricting usage to a single operating system was never considered. With the advent of cross-platform GUI libraries such as the *Fast Light Toolkit (FLTK)* (Spitzak, 2004), it became possible to create a GUI compatible with Windows, Linux and later Mac OS X. The graphics of *FLTK* are not 'flashy'; however, the library is very small and it is possible to link pre-compiled binaries with a static version, while keeping the executable file size relatively small. The command-line version of *DRAWxtl* is still maintained, and can be built with or without on-screen graphics. The former is used with a graphical shell that integrates well with drag and drop operations on a Mac. The version without graphics is intended to be embedded in other applications as a graphics-generation engine.

2. Input

For a program to generate crystal structure graphics, two forms of data are required. The first is a basic description of the structure, including unit cell, space group, atomic coordinates and displacement parameters. In *DRAWxtl*, the structural information can be input in a number of ways, including (a) a native format, (b) a file in the crystallographic information file (CIF) format, (c) a file in the Cambridge Structural Database (CSD) format, (d) a *GSAS* (Larson & Von Dreele, 2004) input file, (e) a file in the *SCHAKAL* (Keller, 1997) format, (f) a *SHELX* (Sheldrick, 1997) input file, (g) a *DISCUS* (Proffen & Neder, 1997, 1999) file and (h) a *WIEN2k* (Blaha *et al.*, 1996) input file. This number of external formats is supported to reduce the need to retype any structural information. In particular, the choice of CIF and CSD formats provides an interface to the major databases of both inorganic and organic structural chemistry.

The second type of input describes the structural entities to be drawn and technical aspects of the production of the graphics. This information is always input using the native format, which consists of

Table 1Sample input file for *DRAWxtl*.

```

title Buckyball
rem specify the crystal structure
cell 14.16
spgp F m 3
atom c 1 0.04908 0.00000 0.24510
atom c 2 0.10028 0.08284 0.21346
atom c 3 0.18313 0.05120 0.16226
rem specify output components and drawing details
sphere c 0.400 Red
bond c c 0.100 1.200 1.550 Gray20
pack 0.045 0.050 -0.01 0.01 0.24 0.25
molcomp 1.60
origin 0.00 0.00 0.00
box 0.000 Black
axislines 0.00 White
nolabels
view -12.7 -0.5 -0.6
phong 0.10 10.00
end

```

free-format data starting with a keyword that describes the type of information that is being supplied. Except for the end and the frame line, the order of these items is unimportant. Use of the frame line will be discussed later. Table 1 contains the input file to produce a drawing of one molecule of C_{60} , with the *POV-Ray* rendered output shown in Fig. 1. For purposes of illustration, the commands that describe the structure are separated from those that control the drawing, but they could be input in any order. A symmetry-generator routine adapted from that of *LAZY PULVERIX* (Yvon *et al.*, 1977) is used to generate the transformation matrices for any space group from the Hermann–Mauguin symbol.

The commands in Table 1 are mostly self-explanatory. Because the structure is cubic, we only have to specify the length of the a axis, which may be in Å or pm, whichever is preferred. All other distances must be given in the same units as the unit cell. The atom lines specify the three distinct types of C atoms in the idealized buckyball structure. In the section that describes the drawing, we specify that C atoms are to be the centers of red spheres of 0.4 Å radius, and that bonds of 0.1 Å radius are to be drawn in a dark gray between C atoms that are between 1.1 and 1.5 Å apart. The pack command gives the x , y and z ranges in fractional coordinates of the atoms to be plotted, relative to the origin. Note that this range just encompasses the position of atom C1. The molcomp command recursively includes any atoms within 1.6 Å of any atom already in the diagram to complete the molecule. In this case of a compact, isolated molecule, it would

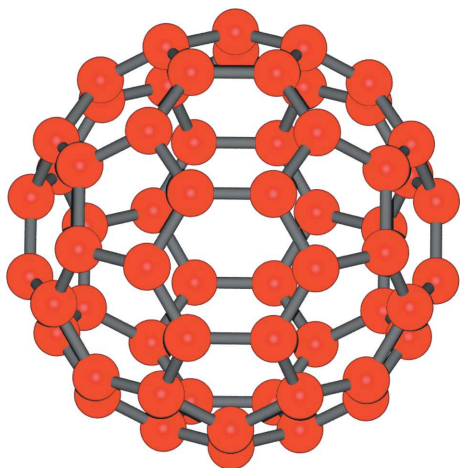
**Figure 1**

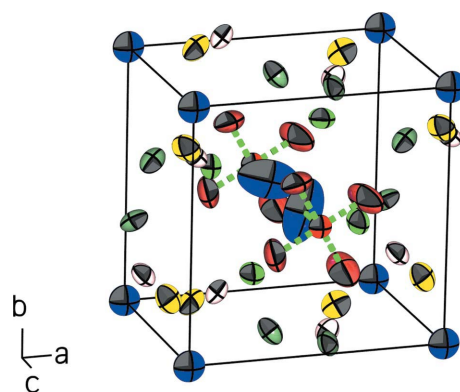
Diagram produced from the commands in Table 1.

have been equally valid to have increased the limits in the pack command to encompass the molecule completely at the origin. For interacting molecules or extended structures, either method may be preferable depending on the task at hand, and the program also provides for deleting excess atoms or fragments by interactive selection or placement of a freely definable, oblique box around the region of interest. The origin command specifies the origin of the figure, overriding the default value of (0.5, 0.5, 0.5). The next several commands turn off the drawing of the unit cell and prevent the automatic labeling of the axes. The view command specifies the orientation of the unit-cell axes relative to the view direction, and the phong command sets the size and brightness of the light reflections from the spheres when rendered in *POV-Ray*.

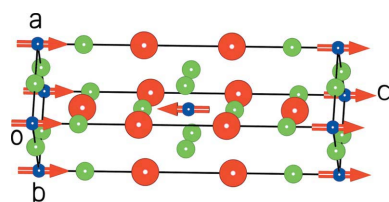
3. Standard drawing elements

As shown in the previous section, *DRAWxtl* can create ball-and-stick diagrams. It can also draw displacement ellipsoids with or without one octant removed, as shown in Fig. 2, which displays one of the *SHELX* sample problems where ellipsoids are drawn at the 50% probability level. Bonds may be shown solid or dashed, and bonds extending beyond the chosen view box can be drawn truncated to emphasize the extended nature of the structure. The vector triple showing the unit-cell axes is optional. The program attempts to place this triple in a location that is not obscured; however, we have not achieved a fail-proof algorithm. Accordingly, the user may drag the vector triple and its labels to any desired part of the screen. Similarly, each of the labels may be repositioned individually.

For representation of magnetic moments or other directional quantities, *DRAWxtl* has the ability to draw arrows, as shown in Fig. 3, which shows the magnetic spin moments of K_2NiF_4 . The program can handle more complicated cases where the spin axes do not line up with the unit-cell axes, or where the magnetic unit cell is a multiple of that defined by the symmetry of the nuclei.

**Figure 2**

Ball-and-stick diagram of displacement ellipsoids with one octant removed.

**Figure 3**Structure of K_2NiF_4 showing the spin magnetic moments as arrows.

computer programs

Table 2

Graphics commands used to generate the lone-pair electron representation for Cs_3SbO_3 .

```
bond SB 0 0.100 1.600 2.400 Gray30
sphere SB 0.300 Gray10 filter 0.5
sphere O 1 0.350 NavyBlue
lonepair SB 1 2.000 0.075 0.300 NeonBlue
pack -0.10 0.15 -0.10 0.15 -0.10 0.15
```

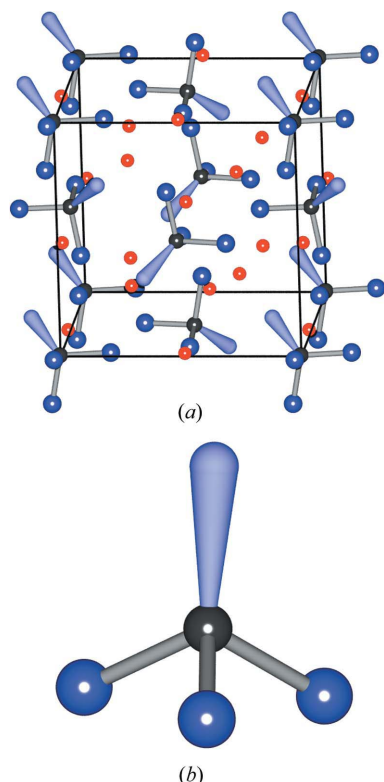


Figure 4

(a) The packing diagram of the structure of Cs_3SbO_3 (Emmerling & Röhr, 2001) with lone pairs located and drawn. (b) A detail of the pseudo-tetrahedron of three O atoms and two lone-pair electrons about Sb.

For structures that include lone-pair electrons, *DRAWxtl* has a facility that will locate and draw a tapered cone capped with a half-sphere to indicate the location and direction of the lone pairs. Fig. 4(a) is a drawing of the structure of Cs_3SbO_3 (Emmerling & Röhr, 2001) with lone pairs displayed. Fig. 4(b) shows an enlarged view of the pseudo-tetrahedron of three O atoms and one lone pair about Sb. To generate the latter graphic, the structure-generation commands in Table 2 were used. The `lonepair` command draws a single lone pair about the Sb atoms with the cone height at 2.0 Å and the taper ranging from 0.075 Å at the originating point and 0.30 Å at the end away from Sb. The `filter 0.5` part of the `sphere` command for Sb sets the transparency of this sphere at 50%.

Mineralogists and others that study inorganic crystal structures are frequently more interested in polyhedral representations than in ball-and-stick diagrams. To satisfy this need, *DRAWxtl* can draw polyhedra of any complexity determined by selection of atom types for the central and vertex atoms, and specification of a maximum coordination distance or both minimum and maximum distances; this allows the display of concentric coordination shells. The program can also draw planar coordination environments, such as would be found for carbonates or borates, and best fitting planes through groups of atoms. For each polyhedron that is displayed, the volume is calculated

Table 3

Essential commands to generate frames with different space groups.

```
title example of different space groups in frames
cell 10.426728 15.003650 8.846367 90 105.7385 90
spgp C 1 m 1
atom SI 1 0.651900 0.240791 0.113936
atom SI 2 0.702092 0.397987 0.671102
....
atom O 20 -0.718070 0.500000 -0.681404
edges 0.02 Black
sphere O 0.300 Yellow
polysz SI 2.000 Green
pack -0.10 1.10 -0.10 1.10 -0.10 1.10
frame
spgp C 1 1 1
atom C 21 0.443223 0.023265 0.291413
atom D 22 0.411059 0.089601 0.242653
....
atom D 29 0.599284 0.096371 0.634512
finish 0.70 0.30 0.080 0.01
bond C C 0.0500 1.000 2.000 Black
bond C D 0.0500 0.7000 1.5000 Black
sphere D 0.2000 Red
sphere C 0.200 Blue
pack -0.10 1.10 -0.10 1.10 -0.10 1.10
end
```

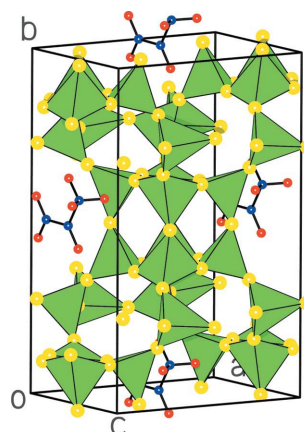


Figure 5

The silicate framework of zeolite ITQ-12 ($\text{Si}_{24}\text{O}_{48}$) with low-symmetry adsorbed propene (C_3D_6) molecules in the cavities (Yang *et al.*, 2005).

and printed. In addition, the quadratic elongation and angle variance, key quantities that describe regularity (Robinson *et al.*, 1969), are output for tetrahedra and octahedra. At the discretion of the user, the corners of polyhedra may be represented by spheres or ellipsoids, or left unadorned. In the *POV-Ray* version of the output, the transparency of the component planes of the polyhedra may be adjusted, allowing visibility of internal features.

4. Advanced drawing elements

One of the features of *DRAWxtl* is a concept called 'frames', which allows the combination of several different structures, each having its own set of parameters including atom descriptions and/or space group, and displays them in the same diagram. Fig. 5 shows the results of a combined synchrotron and neutron diffraction study of the deuterated propene (C_3D_6) adsorption sites in zeolite ITQ-12 ($\text{Si}_{24}\text{O}_{48}$) by Yang *et al.* (2005). The zeolite framework crystallizes with space group *Cm*. The sites for the adsorbed molecules have a symmetry that deviates only slightly from *2/m*; however the molecules have lower symmetry. The drawing was produced with the commands

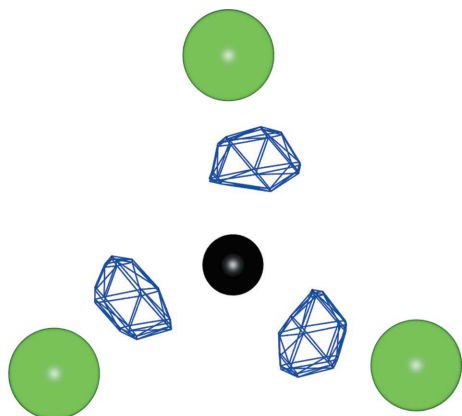


Figure 6
Electron density mesh contour at $0.35 \text{ e } \text{Å}^{-3}$ in the bonds between boron (small sphere) and oxygen in the painite ($\text{CaZrB[Al}_9\text{O}_{18}]$) structure (Armbruster *et al.*, 2004).

in Table 3. The input data are divided into sections using the `frame` command. Each section has its own atoms, space group and drawing limits. In this manner, the orientation of the adsorbed molecules can be shown without having any disorder complicate the diagram, nor is the user required to generate the silicate framework in a lower-symmetry space group. The `frame` command is also useful to allow different sections of a structure to be drawn with different representations, for example, to combine a ball-and-stick and polyhedral plots. Note that when a `frame` command is used, commands become grouped within `frame` units, but their order within those units remains arbitrary.

Another feature of *DRAWxtl* is its ability to combine the solid or mesh contours of a Fourier map with the drawing of the crystal structure. The marching cubes algorithm (Lorenson & Cline, 1987), as implemented by Polyakov (2002), is used to locate the desired surface in the map. This capability is highlighted in Fig. 6, which shows the electron density in the vicinity of the B-O bonds in the painite ($\text{CaZrB[Al}_9\text{O}_{18}]$) structure (Armbruster *et al.*, 2004). The map information may be read from experimental electron density files created by the *FullProf* (Rodríguez-Carvajal, 2001), *GSAS* (Larson & Von Dreele, 2004) and *JANA2000* (Petříček & Dušek, 2004) programs, or from theoretical data calculated by the *WIEN2K* (Blaha *et al.*, 1996) or *VASP* (Kresse & Furthmüller, 1999) codes. An absolute or difference Fourier electron density map can also be computed directly from *SHELX* structure factors in *SHELX* format.

A unique feature of *DRAWxtl* is the ability to draw the structures of aperiodic structures with one-, two- or three-dimensional modulations. The currently supported modulating functions are those defined in version 1.0.1 of the modulated and composite structures CIF dictionary, *msCIF* (Madariaga, 2005), with the exception of rigid groups. Besides harmonic modulation functions for positions, occupancies and displacement parameters, this includes the sawtooth function (Petříček *et al.*, 1990) for positional modulation and the block-wave or crenel (Petříček *et al.*, 1995) function for discontinuous modulation of occupancies. *DRAWxtl* can then only draw those atoms where the occupancy exceeds a specified threshold value or can scale the radius of individual atomic spheres according to the occupancy.

In addition, the program can handle composite crystals (van Smaalen, 1991), as shown in Fig. 7, which is a drawing of the structure of lévyclauidite-(Sb) by Evain *et al.* (2006). This (3+2)-dimensional

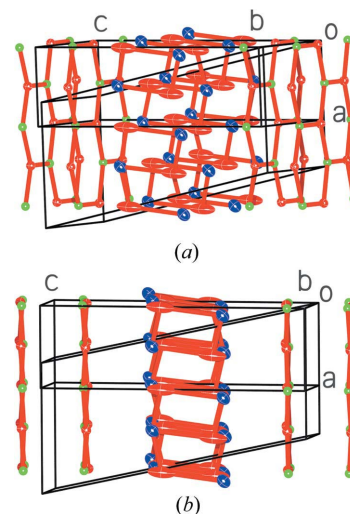


Figure 7
Structure of the composite crystal of lévyclauidite-(Sb), $(\text{Pb}_{0.701}\text{Sb}_{0.299}\text{S})_{1.357}(\text{Sn}_{0.851}\text{Cu}_{0.299}\text{S}_2)$, a (3+2)-dimensional modulated structure. (a) Unit cells for the two components show significant mismatch, particularly along the *b* axis. (b) If the structure were periodic, the CuS_2 sheets would be parallel to the *ab* plane.

structure is interpreted as 'the combination of two heavily modulated triclinic subsystems with a common \mathbf{q} wavevector and only one shared reciprocal axis'. This mineral is a member of the cylindrite family, which crystallizes in thin sheets that roll into cylinders. Fig. 7(a) shows the lattice mismatch between the two components, which leads to the distortion. The aperiodicity of the modulated structure is seen in Fig. 7(b). In the average structure, the sheets containing Cu and S are parallel to the plane containing *a* and *b*, but not in the modulated structure. At present, modulation data can only be entered using a CIF.

In addition to the standard *POV-Ray* output, *DRAWxtl* also includes the capability to insert the special commands needed for program *StereoPOV* (Voßeler, 2003) to produce image pairs for conventional or cross-eyed stereoscopic viewing.

4.1. Graphical User Interface

A screen shot of the *DRAWxtl* GUI is shown in Fig. 8. On the right-hand side is the live OpenGL window, which displays the current state of the drawing. This view is reproduced in the *POV-Ray* output on request or exit. Using the computer's pointing device as a virtual trackball, this view may be oriented as desired. The text boxes and 'spinners' on the left-hand side of the screen control the range of plotted atoms and the scale of the drawing. The parameters for other objects such as spheres, ellipsoids, polyhedra *etc.* are controlled by edit screens such as the one shown. As an aid to the user, the entire program manual may be viewed on screen through various help screens.

4.2. Obtaining the program

This open-source program, written in C and C++, may be freely downloaded from <http://www.lwfinger.net/drawxtl>. In addition to the source, the web site also contains pre-compiled binaries for Windows (9X, NT, 2000 and XP) as a self-installing executable, Mac OS X (G4/G5) as a compressed-disk image file, and Linux (i386 only) as a compressed-tar archive. Also included with each form of the distribution is a machine-readable copy of the program manual and a set of sample input files.

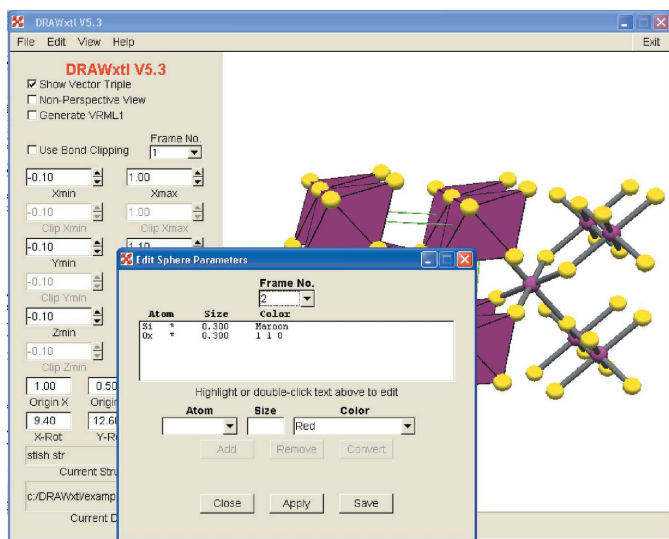


Figure 8

A screen shot of the *DRAWxtl* GUI showing the live OpenGL picture of the structure. The extent of the drawing and the centering are controlled by the text box and spinner widgets on the main page, while the various objects such as spheres are modified through edit screens as shown. The full program manual is available through the Help menu.

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