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

Larry W. Finger, Martin Kroeker and Brian H. Toby
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.

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 SHELeX (Shekridck, 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 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.

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 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.
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.

### Table 1

Sample input file for DRAWxtl.

```
title Buckyball
rem specify the crystal structure
molcomp 1
origin 0
box 0
pack 0

atom c 1 0
atom c 2 0
atom c 3 0

rem specify output components and drawing details
molcomp 1.60
origin 0.00 0.00 0.00
box 0.000 1.000 1.560 Gray20

rem specify drawing frame
pack 0.045 0.050 -0.01 0.01 0.24 0.25

rem specify drawing frame
molcomp 1.60
origin 0.00 0.00 0.00
box 0.000 1.000 1.560 Gray20

rem specify drawing frame
pack 0.045 0.050 -0.01 0.01 0.24 0.25

rem specify drawing frame
molcomp 1.60
origin 0.00 0.00 0.00
box 0.000 1.000 1.560 Gray20

rem specify drawing frame
pack 0.045 0.050 -0.01 0.01 0.24 0.25
```

### 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 $\text{K}_2\text{NiF}_4$. 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.
computer programs

Table 2

<table>
<thead>
<tr>
<th>Graphics commands used to generate the lone-pair electron representation for Cs3SbO3</th>
</tr>
</thead>
<tbody>
<tr>
<td>bond SB D 0.100 1.600 2.400 Gray30</td>
</tr>
<tr>
<td>sphere SB 0.300 Gray10 filter 0.5</td>
</tr>
<tr>
<td>sphere O 1 0.350 NavyBlue</td>
</tr>
<tr>
<td>lonepair SB 1 2.000 0.075 0.300 neonBlue</td>
</tr>
<tr>
<td>pack –0.10 0.15 –0.10 0.15 –0.10 0.15</td>
</tr>
</tbody>
</table>

Table 3

<table>
<thead>
<tr>
<th>Essential commands to generate frames with different space groups</th>
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</thead>
<tbody>
<tr>
<td>title example of different space groups in frames</td>
</tr>
<tr>
<td>cell 10 426728 15.003650 8.446387 90 105.7385 90</td>
</tr>
<tr>
<td>spgp C 1 m 1</td>
</tr>
<tr>
<td>atom SI 1 0.651900 0.240791 0.113936</td>
</tr>
<tr>
<td>atom SI 1 0.702092 0.397987 0.671102</td>
</tr>
<tr>
<td>...</td>
</tr>
<tr>
<td>atom D 20 –0.718070 0.500000 –0.681404</td>
</tr>
<tr>
<td>edges 0.02 Black</td>
</tr>
<tr>
<td>sphere O 0.300 Yellow</td>
</tr>
<tr>
<td>polyz3 SI 2.000 Green</td>
</tr>
<tr>
<td>pack –0.10 1.10 –0.10 1.10 –0.10 1.10</td>
</tr>
<tr>
<td>frame</td>
</tr>
<tr>
<td>spgp C 1 1 1</td>
</tr>
<tr>
<td>atom C 21 0.443223 0.023265 0.291413</td>
</tr>
<tr>
<td>atom D 22 0.410559 0.089601 0.242663</td>
</tr>
<tr>
<td>...</td>
</tr>
<tr>
<td>atom D 29 0.599284 0.096371 0.634512</td>
</tr>
<tr>
<td>finish 0.70 0.30 0.080 0.01</td>
</tr>
<tr>
<td>bond C C 0.0500 1.000 2.000 Black</td>
</tr>
<tr>
<td>bond C D 0.0500 0.7000 1.5000 Black</td>
</tr>
<tr>
<td>sphere D 0.2000 Red</td>
</tr>
<tr>
<td>sphere C 0.200 Blue</td>
</tr>
<tr>
<td>pack –0.10 1.10 –0.10 1.10 –0.10 1.10</td>
</tr>
<tr>
<td>end</td>
</tr>
</tbody>
</table>

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 Cs3SbO3 (Emmerling & Rohr, 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%.

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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 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 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 (C3D6) adsorption sites in zeolite ITQ-12 (Si24O60) 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 4
(a) The packing diagram of the structure of Cs3SbO3 (Emmerling & Rohr, 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.

Figure 5
The silicate framework of zeolite ITQ-12 (Si24O60) with low-symmetry adsorbed propene (C3D6) molecules in the cavities (Yang et al., 2005).
in Table 3. The input data are divided into sections using the fframe 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 fframe 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 fframe 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 (Lorensen & Cline, 1987), as implemented by Polylakov (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 (CaZrB\([Al_9O_{18}]\)) structure (Armbruster et al., 2004). The map information may be read from experimental electron density files created by the FullProf (Rodriguez-Carvajal, 2001), GSAS (Larson & Von Dreecle, 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, mCIF (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 lévy-claudite-(Sb) by Evain et al. (2006). This (3+2)-dimensional structure is interpreted as ‘the combination of two heavily modulated triclinic subsystems with a common 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 (Voželar, 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.
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References