to create drawings with separate parts of the diagram having different contents, or even different space groups.

As shown below, V5.0 implements a full-featured GUI that uses the Fast Light Tool Kit (FLTK). Not only is the structure drawing rendered as in V4.1, but also parameters of the structure and the diagram can be modified and the changes viewed in real time. In this multi-frame diagram of stishovite, one of the new capabilities of the frame command is demonstrated by composing the left-hand unit cell with SiO_6 octahedra; whereas the right-hand portion is drawn with balls and sticks. The main screen includes widgets to set the overall limits of the diagram and a few other parameters; whereas the pull-down menus are used to access structural elements such as polyhedra, bonds, etc. Complete on-line help is also available.
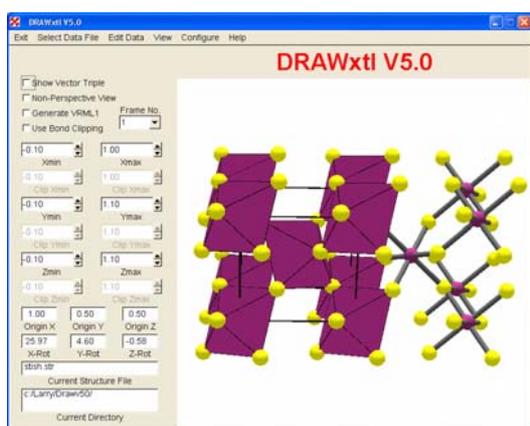
Below, is a representative of the edit windows, is a screen shot of the window used to edit polyhedra and planes. To help in setting the minimum and maximum distances for the polyhedron, the "To" interatomic distances are shown in the combo box. Whenever a particular line in that box is highlighted, the appropriate data are transferred to boxes 'From', 'To', etc. Once all these items are non-blank, the

program activates the 'Add' button. When this button is pressed, the data are transferred into the upper window. Alternatively, the data in the window can be edited directly. Once the data have been adjusted as desired, either the 'Apply' or 'Save' is pressed. At that time, the changes are shown in the main-screen display. The 'Frame No' combo box is shown and active whenever the data file contains more than one frame.
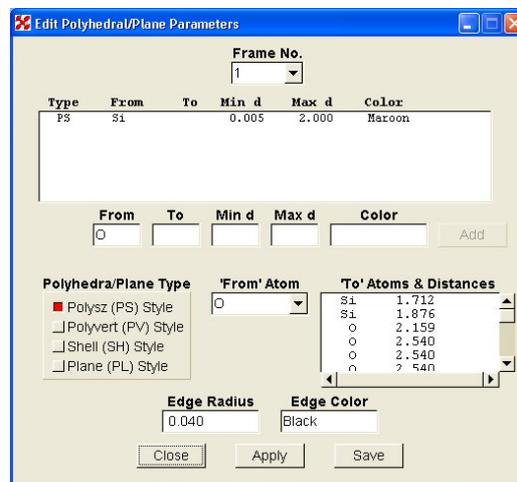
Obtaining the Program

As before, the new versions of DRAWxtl run under Linux, other Unix derivatives, and Windows (9X, Me, XP, NT, and 2000). In addition, a port of the programs to Mac OS X is in progress at the time of this writing. The source code, executable programs for Windows (and OS X?), sample data sets, and the manual are available from http://www.lwfinger.net/drawxtl. DRAWxtl is open-source software, and is free to anyone. We hold copyright on the code, and like any other piece of intellectual property, we ask that you respect our rights.

XtalDraw for Windows

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The XtalDraw suite of crystallographic software for Windows is freely available from the website http://www.geo.arizona.edu/AMS/amcsd.php. The program reads crystal structure data and produces interactive images of the structure rendered as ball and stick, polyhedral or displacement ellipsoids. When initially drawn, the crystal structure is oriented with **c*** coming out of the screen and the **b**-axis horizontal, just like the International Tables. The images can be rotated with the arrow keys, or oriented in specific crystallographic directions through a dialog box interface. The image can be resized by hitting the +/- keys or by specifying a certain image width.
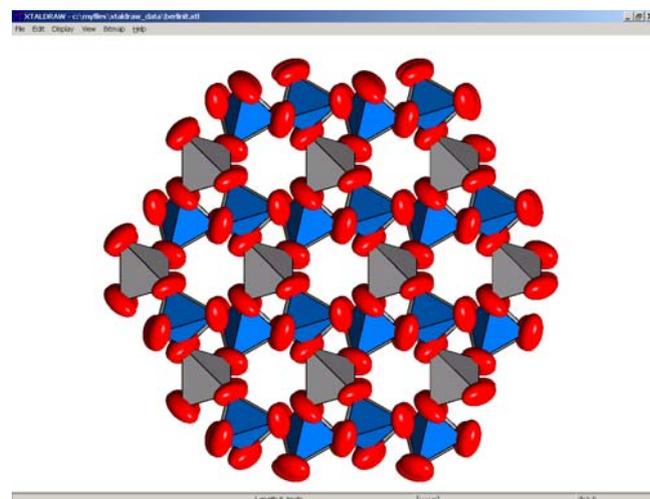

Fig. 1: *Structure of Berlinite (Aluminium Phosphate) as generated by Xtal Draw.*

Default atom colors are chosen to match Lipson and Cochran (1957) and sphere radii are scaled to Shannon and
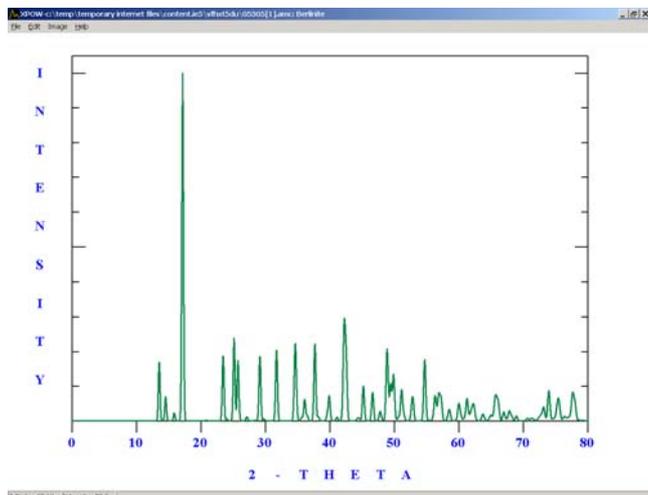
Fig. 1: *Powder diffraction pattern of generated by Xtal Draw.*

Prewitt (1969). The user can easily alter these and new defaults can be established. If the data permits, then displacement ellipsoids can be drawn. The user can alter the probabilities associated with the ellipsoids and thus change their sizes. Initially, a complete unit cell of the crystal is drawn. The extent of the drawing can be altered in several interactive ways.

A useful feature of the software is the ability to make animations of the images created with the program. This feature permits the study of crystal structure behavior as a function of some arbitrary parameter of interest, such as temperature, pressure, dehydration, and so on. The images can be easily ported into gif89 freeware, such as Gamani Movie Gear, to create animations for the Internet or for PowerPoint presentations.

The software also computes several important crystallographic parameters that are presented in ASCII files, such as bond lengths, angles, polyhedral volumes, distortions, displacement ellipsoid and thermal motion TLS rigid body analysis. Furthermore, powder diffraction profiles can also be computed from the crystal structure data in an interactive fashion, with user defined radiation sources, limits and peak widths.

Perhaps one of the important aspects of the software that separates it from others is that it is intimately linked to a free online database, The American Mineralogist Crystal Structure Database at http://www.geo.arizona.edu/AMS/. This database currently contains the crystal structure data for every crystal structure published in the American Mineralogist, The Canadian Mineralogist, the European Journal of Mineralogy and Physics and Chemistry of Minerals, and the process of adding structures from Acta Cryst has just been initiated. The database has ~7000 datasets right now. It is jointly maintained by the American, Canadian, German and European mineralogical societies. After the XtalDraw software has been installed from the Database website, then searches on the website produce hyperlinks that automatically download the dataset by ftp and open it directly into XtalDraw for the users pleasure.

STRUPLO 2004:
A new version of the structure drawing program

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The crystal structure drawing program *STRUPLO*, initially programmed in FORTRAN [1] is completely rewritten in Delphi and redesigned with extensive modifications and new options. It is part of the *BRASS* (The Bremen Rietveld Analysis and Structure Suite) program package [2,3]. The main features are:

- Bitmap graphics
- Bonds can be drawn as cylinders, atoms as spheres
- Atoms are drawn with their predefined ionic radius. The size of cations and anions can be scaled separately or individually.
- Polyhedra are identified within a sphere of given radius between the central atom and the ligands
- Fast online rotation
- Online identification of any element (atom, bond, polyhedron)
- Each of the elements can be deleted and undeleted at any time
- Online distance and angle calculation, complete table of distances and angles
- Attributes (e.g. color, transparency, atom size etc.) can be assigned to all items, to chemical elements, to single atoms in the asymmetric unit, or to any single atom or item.
- Symmetry operators are generated from space group symbol (routine [4] translated to Delphi) with origin shift for nonstandard space groups.
- The void space, i.e., the empty space not occupied by atoms, is calculated according to the procedure described in [5]. This is especially useful to determine diffusion paths, e.g., in porous materials like zeolites.

The following figures show a screen print of a typical page in the user interface (Fig. 1) and several examples of projections of zeolite A [6] in various representations.