DRAWxtl 5.1 - A Multi-Platform Computer Program to Display Crystal Structures

Martin Kroeker[a], Brian H. Toby[b], Larry W. Finger[c], [a]*Department of Inorganic Chemistry, University of Freiburg, Germany.* [b]*NIST Center for Neutron Research, Gaithersburg,USA.* [c]*Geophysical Laboratory,Washington D.C., USA(retired).* E-mail: martin@ruby.chemie.uni-freiburg.de

The computer program DRAWxtl is designed to display a crystal structure with minimal user input and maximum flexibility. It reads the description of a crystal structure, including unit-cell parameters, space group, atomic coordinates and thermal parameters, combines them with options that define the view, and outputs a geometry object that may contain polyhedra, planes, lone-pair cones, spheres or ellipsoids, bonds, and the unit-cell boundary lines.

Since the recently released version 5.0, the program presents an easy to use graphical user interface where the drawing can be previewed, and all parameters are accessible through conventient menues or direct interaction. A functionally identical command-line version is still available for easier integration into other program packages that provide their own user interface.

The most prominent new feature in version 5.1 is its ability to import electron density information from GSAS and JANA, which can be rendered as meshes and/or solid surfaces. Using a 3D cursor, local maxima in the electron density can be determined to aid in structure solution and refinement.

Both the complete source code and precompiled binaries for Linux, OSX, MS Windows and Irix are freely available from http://lwfinger.net/drawxtl.

Keywords: graphics, software, crystal structures