

**CrystalMaker 6.3.** CrystalMaker Software, Begbroke Science Park, Building 5, Sandy Lane, Yarnton OX5 1P5, U.K. <http://www.crystallmaker.com>. \$599.00 (single user), \$415.00 (academic, single user). Contact company for other pricing options.

Visualization of a molecule in three-dimensional space can be challenging, especially when the molecule is packed in a crystal where intermolecular interactions must be considered. CrystalMaker 6.3, written by David Palmer of the Earth Sciences Department at Cambridge University, U.K., is designed primarily as a visualization tool. As such, it is a useful teaching aid for beginning students of crystallography as well as for researchers because the program displays molecules well and quickly. It is excellent for promoting understanding of crystal packing and bonding information. In addition, the program is user-friendly, and with the guidance of the manual, students can explore molecules from different crystal classes from the 150 data files provided.

CrystalMaker was written and exclusively designed for the Macintosh computer running OS X v. 10.1.2 or later. Having a large computer monitor is preferable since multiple windows will be open while the program is running. The program was easily installed, and it is compatible with input from many commonly used data formats: CCL, ChemBats3D, CIF, CSSR, MacMolecule, PDB, SHELX, and CDB, etc. The program follows the usual Mac convention of pull-down menus. In addition, it has several uncommon icons that give convenient access to on-screen operation.

The modeling options provided are ball-and-stick, space filling, polyhedral, wire frame, and stick. The ball-and-stick and space-filling options produce beautiful images. One can also choose to display only part of the molecule of interest. It is possible to visualize atomic radii with atomic, covalent (tetrahedral or octahedral), crystal atomic, or CDB atomic, and users can choose the type of radii and colors of the atom interactively. Entering the data for a new crystal is easy. However, the surface

option is a bit confusing: instead of displaying the molecular surface, the surface that is shown looks just like the space-filling model but with different materials.

Using the program is easy for neophytes, and the documentation is clearly written and illustrated. Most of the function keys are intuitive. My collaborators and I also tried the tutorial in which everything worked except the bond-making function: the number of bonds that were displayed between Mg–O in  $\text{MgAl}_2\text{O}_4$  did not match the number of bonds that were made with the “Edit” function; that is, only two of the four bonds were displayed.

One attractive feature of this program is that the manipulation of the molecule is recorded in the “history”, so that one can easily backtrack to a specific step. In addition, we liked having the ability to write notes next to the display window. We did find, however, that the speed of the program was reduced when a large molecule was loaded. We loved the display of crystal packing: one of the difficulties in teaching crystallography to beginning crystallographers is getting them to imagine crystal packing; with the aid of CrystalMaker, students can visualize the different symmetries and molecular packing in different space groups.

In conclusion, CrystalMaker 6.3 is a very powerful tool for display and teaching. This version is more versatile with the input and output file formats than its predecessors and interfaces with other crystallographic programs more readily. The price of \$599.00 for the general single user and \$415.00 for the single academic user, though, seems a bit high considering that there are several analogous programs available to academic users that are free of charge.

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