JCE Featured Molecules

edited by
William F. Coleman
Wellesley College
Wellesley, MA 02481

Molecular Models of Crystalline Materials

TiO_2 and Copper Compounds

August 2009 Featured Molecules

The featured molecules for this month come from two papers dealing with crystalline materials. In the first paper, Supan Yodyingyong, Bhinyo Panijpan, Wannapong Triampo and Darapond Triampo present an inexpensive method for synthesizing nanocrystalline TiO_2 *(1)*. In the second paper, Bodie Douglas applies the methods that he has developed based on layers and packing arrangements to the structures of four copper salts, demonstrating subtleties of structure that may not be readily apparent on examination of the unit cell structure *(2)*.

The visualization of solid state structures is quite difficult for many students, and it is essential that they have access to as many tools as possible to aid them in this effort. Some students find images on paper, no matter how carefully constructed, to be very confusing, and the more information that is presented in the image in an effort to aid understanding, the more confusing they find it. Building models, using for example the ICE Solid State Model Kit, helps many students see structures in ways that they cannot with only flat images *(3)*. There are obviously other approaches to building tactile models ranging from gumdrops and toothpicks to large "Styrofoam" balls and sticks.

Ready access to molecular viewers makes it possible to construct and view many rotatable, scalable, and customizable structures in a relatively short time. Like other computer and Web-based applications, these structures are available to students at any time, and allow them to study structures until they gain some mastery of the material at hand.

Structures can be built using a number of programs, including HyperChem *(4)*, GaussView *(5)*, and CrystalMaker *(6)*. As Douglas points out, a demonstration copy of CrystalMaker is freely available, but structures cannot be saved *(6)*. Using these tools introduces students in more advanced undergraduate courses to space group symmetry, Hermann–Mauguin notation, Miller indices, fractional coordinates, and other topics.

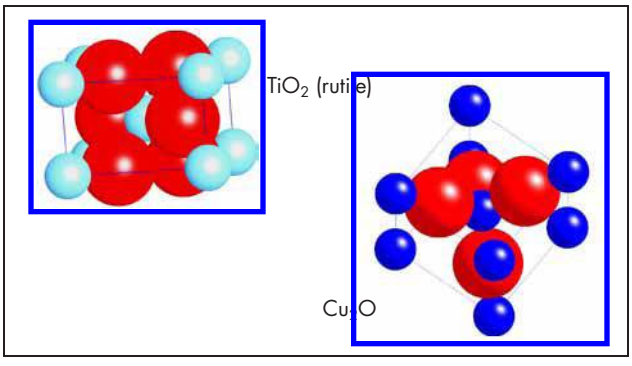

Figure 1. Two of the molecules added to the *JCE* Featured Molecules collection this month: TiO_2 *(1)* and Cu_2O *(2)*.

There are also a number of free online sources of crystallographic data in the form of files that can be read by these programs, or read as text files with hand entry of unit cell parameters *(7)*. Additionally, a number of Jmol-enabled sites now focus solely on crystal structures, providing students with a very large array of structures to explore and enhance their understanding and teachers with many possibilities for examples and assignments *(8)*. Recent versions of Jmol have added a variety of tools for exploring crystal structures, including the ability to add planes, identify the space group, etc. *(9)*.

Included in this month's structures are the three polymorphs of TiO_2, rutile, anatase, and brookite, and various views of structures from the Douglas paper (Figure 1).

Literature Cited *(all sites accessed Jun 2009)*

1. Yodyingyong, S.; Panijpan, B.; Triampo, W.; Triampo, D. *J. Chem. Educ.* **2009,** *86,* 950–952.
2. Douglas, B. *J. Chem. Educ.* **2009,** *86,* 980–984, and references therein.
3 Mayer, L. A.; Lisensky, G. C. Solid State Model Kit. Institute for Chemical Education (ICE) Publication 92-004. *http://ice.chem.wisc.edu/Catalog/SciKits.htm#Anchor-Solid-31140*.
4. HyperCube, Inc. *http://www.hyper.com/*.
5. Gaussian.com. *http://www.gaussian.com/index.htm*.
6. CrystalMaker Software. *http://www.crystalmaker.com/index.html*; CrystalMaker Software Downloads. *http://www.crystalmaker.com/downloads/index.html*.
7. Two such sites are: American Mineralogist Crystal Structure Database at *http://rruff.geo.arizona.edu/AMS/amcsd.php* and Crystallography Open Database at *http://www.crystallography.net/*.
8. Such sites include American Mineralogist Crystal Structure Database at *http://rruff.geo.arizona.edu/AMS/amcsd.php* and Exploring the Nanoworld at *http://mrsec.wisc.edu/Edetc/pmk/index.html*.
9. Jmol Interactive Script Documentation. *http://chemapps.stolaf.edu/jmol/docs/*.

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Supplement
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The molecules added to the collection this month are:
three polymorphs of TiO_2 (rutile, anatase, and brookite)
various views of structures from the Douglas paper *(2)*