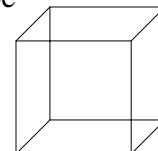


MOLECULAR VISUALIZATION IN BIOLOGY,  
CHEMISTRY, AND GEOLOGY USING CHIME®

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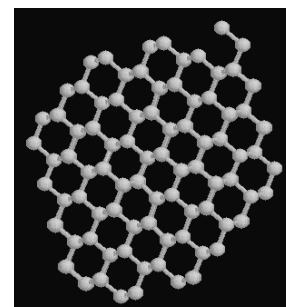
When you look at the shape to the right, what do you see? Are you visualizing a cube, a three-dimensional box made up of 6 square faces or a planar figure? Would your interpretation be different if you could rotate the figure? Do you have students with this problem? If the interpretation of this image presents difficulties, what will happen with complex molecules such as proteins or mineral structures like quartz. How can students visualize these, especially from two-dimensional illustrations on overheads or PowerPoint slides? Remember trying to visualize the shape of a water molecule in chemistry or picture a protein from the page of a biology textbook or figure out the structural difference between diamond and graphite in your geology textbook. If you were lucky, the instructor got the ball and stick models or a pre-constructed model to aid your visualization. Well today, luck is on your side with molecular visualization software that can be installed on your computer. All you need is an Internet connection and Chime, a free plug-in for your browser (Internet Explorer or Netscape). In this article, we will introduce you to the educational benefits of using Chime in your classroom (at a price everyone will love).



Chime, a product of MDL Information Systems, is molecular structure rendering software (freeware) that operates in a browser. Chime Version 2.6 can be downloaded free from <http://www.mdlchime.com/chime> and, when executed, loads into your browser as a plug-in. Once installed in your browser, Chime can read a variety of data file types and convert them to three-dimensional molecular structures that can be manipulated on the screen.

Chime allows you to view a molecular structure from any perspective by “clicking and dragging” to rotate the image. In addition, the display can be changed to view the structure as wireframe, sticks, the ever-popular ball and stick (just like the wooden ones). It can even display structures as space-filled, showing the actual size of the electron clouds around the atoms with packing based on atomic or ionic size.

The Chime rendering of one form of carbon is shown to the right. Is it diamond or graphite? With the crystal structure displayed in your browser, a simple rotation will show it to be diamond, based on the tetrahedral linkage of all the carbon atoms. How easy would it be to achieve this with the orientation of models in the front of the classroom?



**Where do you get the molecular structure files?**

Many structures are readily available on the Internet. An NSF-funded project at Cabrillo Community College has a collection of 400 molecules (and a viewer for Netscape) for downloading (<http://c4.cabrillo.cc.ca.us>). If you enter a molecule name or mineral structure in

a search engine (such as <http://www.google.com>) with chime entered after the name, you will probably locate a number of sites with the desired substance.

### **How do I get my students actively engaged with Chime?**

We have produced a menu-driven interactive student guide to Chime which shows the menu operations to make display changes, remove abundant hydrogen atoms on biological structures, and show transparent electron clouds to view inside structures. The guide also covers measuring bond distances, bond angles, and torsion angles (for the more advanced user). This is available at [http://academic.pg.cc.md.us/psc/chime\\_guide.html](http://academic.pg.cc.md.us/psc/chime_guide.html). You will need Chime installed in your browser to use it. We illustrate the use of Chime in an activity that explores the chemistry of cisplatin and its binding to DNA as an anticancer drug. A number of great websites with Chime applications are given at the end of our guide.

### **Can using Chime dispel molecular misconceptions?**

Many students cannot visualize the three-dimensional nature of structures especially from the two-dimensional presentations used. This can occur with molecules as simple as a tetrahedral methane molecule. The physical models we use (such as the ball and stick), in student kits or larger constructed models, leave an image in student's minds of rigid, very open structures. Using Chime for three-dimensional viewing with the space filling option showing electron clouds can help dispel these misconceptions. The packing of solids is easily shown and viewable within the structure. Chime also has the capabilities to show molecular motion in molecules—stretching, bending, and other movements.

### **How do you insert the molecular structure files that use Chime into a web page?**

If you are a Microsoft FrontPage user, a Chime readable file is embedded from the Insert menu under Advanced under Plug-in. This will open a window to browse for the file and then set the position and size of the image. The images can be viewed in your browser. The browser will display the files from a disk (you do not need to be on the Internet).

If you are a Netscape Composer user, a Chime readable file is embedded from the Insert menu under HTML Tag, where you write a line of HTML code. Here is an example of the code:  
<embed src="Sulfur8.pdb" width="150" height="150" align="right">

You can view a Chime file in the browser directly. If you open your browser, and go to File, select open, and then locate and click on the molecule file, it will be displayed.

If you are not fond of web page designing, RasMol is a similar piece of molecular visualization software that will run off your desktop. It can be downloaded free from <http://www.umass.edu/microbio/rasmol/getras.htm> and is small enough to fit on a 3.5 inch diskette (<350 kB). If you are going to get really serious about Chime or RasMol, you need to visit Eric Martz's website at the University of Massachusetts (<http://www.umass.edu/microbio/chime>).

Chime enhances your ability to display and visualize molecular structures and so is another tool to place in your instructional toolbox, along with the ball and stick models. What an aid to biologists, chemists, and geologists in the classroom!