

Teaching Chemistry using the CCDC Data Base



The Cambridge Crystallographic Data Centre (CCDC) provides a free 500-structure interactive, online database for use in educational applications. Visualization of the structures utilizes the free version of the popular Mercury program (http://www.ccdc.cam.ac.uk/free_services/mercury/). The database is included with the Mercury download. A variety of exercises is available to assist in teaching chemical concepts such as VSEPR, aromaticity, and stereochemistry (http://www.ccdc.cam.ac.uk/free_services/teaching/modules/) that may be used on line or downloaded for local use.

Exercise 1. VESPR Study

Open the Mercury viewer.

Open the teaching subset of the CSD by selecting File in the menu bar, choosing Open, selecting examples, selecting the folder teaching_subset, and choosing the database file teaching_subset.ind. The right column of Mercury should contain a list of 500 files and normally the first file will appear in the workspace.

The molecular model may be rotated on the screen by holding the left mouse button down and moving the mouse.

The size of the image on the screen can be adjusted by holding the right mouse button down and moving the mouse.

The atoms may be identified by selecting Display / Labels / Atoms. In the dialog box that opens select Label by element, click the All button, and click Close.

The rendering of the atoms is “wireframe” by default. Choose Display / Styles and select from wireframe, stick, ball and stick, or spacefilling if you wish a different rendering.

Bond lengths may be measured by choosing Measure Distance in the Picking Mode window, clicking on one atom to generate a yellow circle and clicking on a second atom to generate another yellow circle. The distance will appear in green. Click Clear Measurements to remove the values.

Bond Angles may be measured by choosing Measure Angle in the Picking Mode window and clicking on one end atom, the center atom, and the other end atom to generate three yellow circles. The bond angle will appear in green. Click Clear Measurements to remove the values.

Open your internet browser to:

http://www.ccdc.cam.ac.uk/free_services/teaching/modules/ to see a listing of available teaching modules.

Click the Modules link and the General Chemistry link. Choose the Shape of Molecules: VSEPR Model link.

The module can be used on line by clicking the < or the > button or off line by downloading the .pdf file from the button next to the back and forward buttons. To alternate between the module and the Mercury image, simply use standard Windows techniques.

Read through the Introduction and Objectives sections before moving onto the background reading and specific directions. A summary concludes the module.

Exercise 2. Study a Module of Your Choice

As time permits, work through a couple more modules of interest.