

EDU 111 lab Chemistry Databases

1. BioRad KnowItAll AnyWare



Open your internet browser to:

<http://www.knowitallanyware.com/login.html>

Click in the upper right corner to determine the number of compounds in the database.

Click on Help in the menu to read about available data sets, entering search data, etc.

Comparing Database Information for Propanols

Enter cyclopropanol in the search window and click Search.

How many “hits” do you get for this compound? _____

What types data sets are available for this compound? _____

Enter propanol in the search window and click Search.

How many “hits” do you get for this compound? _____

How many different compounds are included? _____

Is there a data set common between cyclopropanol, 1-propanol, and 2-propanol? _____

Open the common data set for each compound and record the peak data from the table.

Cyclopropanol:

1-Propanol:

2-Propanol:

How could you use these data to identify which propanol might be in a sample of an “Unknown”?

Determination of the Identity of an Unknown

The following data were collected for an organic unknown:

White crystalline powder

IR selected peaks: 2920, 1740, 1700, 1600, 1580, 1500, 1480, 1440, 1375, 1315, 1290, 1240, 1100, 1075, 840, 760, 692

Mass spectrometry selected peaks: 152, 107, 77

¹³CNMR: 169, 156, 128, 120, 114, 64

H1NMR: 4.55, 6.85, 7.20

MP: 98

Enter MP: 95-105 AND MW: 152 in the Search window and click Search.

How many "hits" do you get for this search? _____

Move to the bottom of the window and click the link to Search within Results to refine the search.

Enter C13: 169, 156, 128, 120, 114, 64 in the Search window and click Search.

How many "hits" do you get for this refined search? _____

What is the probable identity of the unknown compound? _____

Enter the name of the compound in the Search window and click Search.

Open each of the data sets for this compound and compare the values to those listed above.

Do you feel confident that you have identified the compound? _____

What is the CAS number for the compound? _____

Structure Search

Click on the link to Advanced Search.

Click Draw a Structure and wait until the JAVA environment loads.

Draw the phenoxyacetic acid $C_6H_5OCH_2COOH$ molecule:

Click the Benzene Ring icon (5th icon in column 2) and click in the workspace.

Click the Draw Bonds icon (2nd icon in column 2). Move cursor over one of the C atoms in the ring so that a green circle appears and click once to form a bond.

Move the cursor to the end of the single bond so that a green circle appears.

Click once to form another bond. Repeat two more times so that a total of four single bonds are in the side chain.

With the cursor still in the same position, click once to form a second bond.

Move the cursor to the center of the new bond so that a green circle appears in the middle of the bond. Click once to form a double bond.

Click the Label Atoms icon (2nd icon in column 1).

Move the cursor over the end of the double bond so that a green circle appears and click. Choose O from the drop down list of atoms.

Move the cursor over the end of the chain and insert an O atom which changes to OH.

Place an O atom at the end of the first bond off the ring.

Click Save and Close.

Click Search. How many "hits" do you get? _____

As you scroll through the results list, why are there so many "hits"?

2. Cambridge Structure Database Teaching Database

Open the Mercury viewer (http://www.ccdc.cam.ac.uk/free_services/mercury/).

Open the teaching subset of the CSD (zipped file available at http://www.ccdc.cam.ac.uk/free_services/teaching/downloads) by selecting File in the menu, choosing Open, and selecting the unzipped 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 atoms may be identified by selecting Display / Labels / Atoms. In the dialog box that opens select Add label, 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.

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

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.

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

Open your internet browser to: http://www.ccdc.cam.ac.uk/free_services/teaching 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.