HyperChem Lite: Building Basics

PA State Standards:
3.7.10.C Apply basic computer operations and concepts.
3.4.10.A Explain concepts about the structure and property of matter.
1.2.11.A Read and understand the central content of informational texts and documents in all academic
        areas.

Background:
HyperChem Lite is a molecular modeling and simulation program that predicts physical and chemical properties of molecules. It can be used to determine bond length, bond angles, and molecular shapes. In this activity, you will practice using program to become familiar with it. Later, you will be able to use the program to investigate some basic concepts about chemical bonding.

Guiding Question:
Please answer the following question before completing the experiment.
1. Can double bonds affect the shape of a molecule? If so, how?

Equipment/Materials:
>   Computer with HyperChem Lite software program installed
>   Mouse
>   Mousepad

Procedure:
Method I: Building Molecules Using "Add H and Model Build"
1. Left (L)-double click on the Draw Icon at the top of the screen (Figure 1). The Element Table dialog box will appear. Left (L)-click on hydrogen on the periodic table. L-click on Properties. Record the atomic weight, atomic radius, electronegativity, and electron configuration of hydrogen on the data sheet.

Figure 1: Draw Icon

2. L-click OK on the properties screen. Close the Element Table dialog box. (The Element Table dialog box may be left open if dragged to the side, which can be helpful if multiple elements are needed.)

3. L-click in the workspace. A hydrogen atom will appear.

4. L-click Build. L-click on Add H & Model Build. A complete hydrogen molecule will appear. (Don't freak out! Your molecule should indeed look like a line at this point. Just keep going – it gets better!)

5. Under Setup, make sure there is a checkmark by Molecular Mechanics; if not, L-click on Molecular Mechanics. (This step is only necessary for building the first model once the program has been opened.)

6. Select Compute, L-click on Geometry Optimization. Select Polak-Ribiere. L-click OK. The hydrogen model is now complete and geometrically correct. **Note: Geometry Optimization must be done for every molecule built!**

7. To add labels, L-click Display, and then L-click Labels. Choose Symbol to label each atom. Repeat and choose other labels, if desired. The bond may also be labeled with length.

8. To use different molecular renderings, L-click on Display, and then L-click on Rendering. Choose a rendering, and then click ok. Repeat to view other renderings. Add Dots may be chosen to show the electron cloud.
    a. Balls and Cylinders is often the best rendering to use.
    b. Stick rendering is best if labels are desired or if building complicated molecules.
    c. F2 will flip between the two most recently used renderings.

9. L-click on the XY Translation Tool (Figure 2). L-click and drag in the workspace to move the molecule around the screen. Place the molecule so that most of it is off the screen.

Figure 2: XY Translation Tool

10. To center the molecule on the screen, press the spacebar.

11. To rotate the molecule in the X and Y planes, first L-click on the XY Rotation Tool (Figure 3). Next, L-click and drag in the workspace to rotate the molecule in any direction.

Figure 3: XY Rotation Tool

12. To rotate the molecule in the Z plane, L-click on the Z Rotation Tool (Figure 4). Next, L-click and drag in the workspace.

Figure 4: Z Rotation Tool

13. To zoom in or out, L-click on the Zoom Tool (Figure 5). L-click in the workspace and drag down to zoom in or up to zoom out.

Figure 5: Zoom Tool

14. Draw a sketch of the hydrogen molecule in the data section.

15. There are a couple of ways to clear the workspace.
    a. L-click on File, and then L-click on New. (Instead, you may click on the New icon.) When asked to save, L-click No.

b. L-click on the Selection Tool (Figure 6). L-click in workspace outside of the molecule; the molecule will turn green. L-click Edit, L-click clear, and then answer Yes.

Figure 6: Selection Tool

Method II: Building Molecules by Connecting Atoms

1. L-double click on the Draw Icon (Figure 1). The Element Table dialog box will appear. Left click on oxygen in the periodic table. L-click on Properties. Record the atomic weight, atomic radius, electronegativity and electron configuration of oxygen on the data sheet.

2. Click OK on the properties screen. Close the Element Table dialog box.

3. The rendering should either be sticks or balls and cylinders.

4. L-click in the workspace to draw an oxygen atom. Right (R)-click on the oxygen atom to erase it. R-clicking on an atom or bond while in draw mode (when the curser looks like the draw icon) will erase it. The screen should now be blank.

5. L-click and drag in the workspace to draw two oxygen atoms connected by a bond. One or both atoms may be drawn first, then click and drag to create the bond. **Note: When drawing bonds between existing atoms, the mouse must be clicked and/or released when the curser is at the center of the atom. Otherwise, more atoms will be drawn accidentally.**

6. To draw the double bond, L-click on the single bond. Erase any mistakes by R-clicking. Repeat steps 4 and 5 until comfortable with the procedure.

7. Select Compute, L-click on Geometry Optimization. Select Polak-Ribiere. L-click OK. The oxygen molecule is now complete and geometrically correct.

8. Draw a sketch of an oxygen molecule in the data section.

9. Clear the workspace. Refer to step 15 under Method I if necessary.

Combining Methods I and II

1. Left double-click on the Draw Icon (Figure 1) to open the Element Table dialogue box. Select carbon. Drag the box to the side or close it.

2. In sticks rendering with Symbols as labels, draw six carbons connected together in a ring; there should be six sides. Refer to previous instructions if necessary. The ring does not need to be uniform in shape.

3. Attach another carbon atom that extends from the ring. The molecule should look something like Figure 7, but it need not be
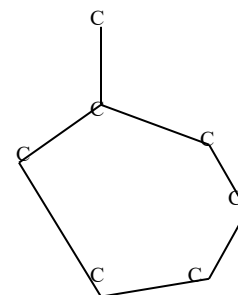
Figure 7

identical.

4. Choose oxygen from the Element Table dialogue box.

5. L-click on the carbon atom that is **NOT** part of the ring to change it to oxygen.

6. L-click on build, and then choose Add H & Model Build.

7. Geometrically optimize the molecule; refer to step 7 under Method II if necessary.

8. Rotate the molecule, cyclohexanol, to view it from different angles; when finished, move it to the side.

9. Once again, build a six-membered ring of carbon atoms with a seventh extending from one of the carbon atoms, as in Figure 7.

10. Alternate double bonds within the ring, as in Figure 8; refer to step 6 under Method II if necessary.

11. Again, change the carbon atom that is **NOT** part of the ring to oxygen.

12. Add H & Model Build. Geometry optimize. This molecule is phenol.

13. Rotate the molecules to examine them from different angles. Observe the differences in shape in the carbon rings.

Figure 8.

14. Sketch both molecules in the data section.

Data:
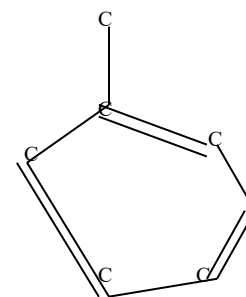
1. For hydrogen, record the: Atomic weight _____.
                                    Atomic radius _____.
                                     Electronegativity _____.
                                    Electron configuration_____.

2. In the space below, sketch a hydrogen molecule.

3. For oxygen, record the: Atomic weight _____.
                                   Atomic radius ____-___.
                                   Electronegativity _____.
                                   Electron configuration_____.

4. In the space below, sketch an oxygen molecule.

5. In the space below, sketch a cyclohexanol and a phenol molecule; show their
    differences in shape. To make this task easier, L-click on Display, and then L-
    click on Show Hydrogens to uncheck it; no hydrogens will be displayed. Show
    the structure of the remainder of the molecule.

Questions:
1. Can double bonds affect the shape of a molecule? If so, how?

2. What command is used to add hydrogen atoms to a molecule, once all other atoms
    have been drawn?

3. What command must be used once a molecule has been completely drawn?

4. Which rendering is best when building complicated molecules?

5. If a molecule has been inadvertently moved off the screen, which key should be
    pressed to return it to the center?

6. What is the procedure for turning a single bond into a double bond?

References:
(Harsh, Hyperchem Lite: Building Basics)
(HyperChem Lite™ Release 2.0 for Windows®, 2003)