

# POLARITY AND MOLECULAR SHAPE WITH HYPERCHEM LITE

## LAB MOD4.COMP

From Gannon University SIM

### INTRODUCTION

Many physical properties of matter, such as boiling point and melting point, are the result of the shape and polarity of the molecules. Both shape and polarity depend on the type of bonding within the atoms. The most common type of bond between two atoms is a covalent bond.

A **covalent bond** is a chemical bond in which electrons are shared between two atoms. There are two types of covalent bonds:

1. Nonpolar-covalent bond - a covalent bond in which the bonding electrons are shared equally by the bonded atoms, resulting in a balanced distribution of electrical charge. The electronegativity, or tendency to attract electrons, in both atoms is the same.
2. Polar-covalent bond - a covalent bond in which the atoms have an unequal attraction for the shared electrons. The atoms have different electronegativities and the electrons have a greater attraction to the atom with the higher electronegativity, causing the bonding electrons being shared unequally and resulting in an unbalanced distribution of electrical charge.

Molecules made up of covalently bonded atoms may themselves be polar or nonpolar. If the polar bonds are symmetrical around a central atom, the bonds offset each other and the molecule is nonpolar. If the polar bonds are not symmetrical, the electrons will be pulled to one end of the molecule and the molecule will be polar.

Another important factor in determining the shape of the molecule is the arrangement of the atoms in space, or molecular geometry. One theory for predicting molecular shape is the **VSEPR** theory, based upon the simple assumption that electrons in molecules repel each other. **VSEPR** stands for “valence-shell, electron-pair repulsion” and states that electrostatic repulsion between the valence-level electron pairs surrounding an atom causes these pairs to be orientated as far apart as possible.

### PURPOSE

The purpose of this experiment is to build models of molecules and predict their polarity based on their shape, using the HyperChem Lite computer software program.

## EQUIPMENT/MATERIALS

Laptop computer with HyperChem Lite installed	HyperChem Lite CD
Wireless Printer and Paper	Ball and stick model kit

## SAFETY


- Keep goggles on hand for use when dealing with glass, chemicals and/or fire.

## PROCEDURE

### The HyperChem Lite Window


1. To start HyperChem Lite, put cursor in the HyperChem Lite Icon, then double click on left mouse. The HyperChem Lite window will open the following list of features:
  - a. Menu Bar: contains the different HyperChem Lite menus which include: File, Edit, Build, Display, Set-up, Compute, Cancel and Help.
  - b. Tool Bar: the left side of the screen contains the tools to draw, select, display and move atoms and molecules.
  - c. Workspace: displays current atoms or molecules.
  - d. Status Line: show a brief description of menu item selected and information about drawing.
  - e. Title Bar: shows name of file working on.
  - f. Control Menu Button: contains commands to move, resize, maximize, and close HyperChem Lite windows. It also contains the switch command, which lets you activate other windows.

### Oxygen Geometry

1. *Left-double click* on drawing icon ()
2. The element table dialog box will appear. *Left-double click* on Oxygen (O) in the periodic table.
3. *Left click* in the workspace. An Oxygen atom will appear.
4. *Left click* Build. *Left click* on Add Hydrogens. A H<sub>2</sub>O molecule will appear.
5. Select Compute, *Left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. H<sub>2</sub>O molecule model is now complete and geometrically correct.
6. *Left click* on Display. *Left click* on Renderings. Select Balls and cylinders, Option, shade and highlighted. *Left click* OK.
7. Measure the bond angle:
  - a. *Left click* on Selection Tool.

- b. *Left click* on Hydrogen and drag cursor to other Hydrogen having oxygen as the apex of the triangle. The bond angle will appear on the lower left below the workspace.
8. Record the bond angle, in degrees, on the Data Sheet.
9. Clear H<sub>2</sub>O molecule from the HyperChem workspace by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.

### **Carbon Geometry**

1. *Left-double click* on the draw icon (). The element table dialog box will appear. *Left-double click* on Carbon (C) in the periodic table.
2. *Left click* in the workspace. A Carbon atom will appear.
3. *Left click* Build. *Left click* on Add Hydrogens. A CH<sub>4</sub> molecule will appear.
4. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. CH<sub>4</sub> molecule model is now complete and geometrically correct.
5. *Left click* on Display. *Left click* on Renderings. Select Balls and cylinders, Option, shade and highlighted. *Left click* OK.
6. Measure the bond angle:
  - a. *Left click* on Selection Tool.
  - b. *Left click* on one hydrogen and drag cursor across to another hydrogen, having the carbon as the apex of the triangle. The bond angle will appear on the lower left below the workspace.
7. Record bond angle for the C-H<sub>4</sub> bond, in degrees, on the data sheet.
8. Clear CH<sub>4</sub> molecule from the HyperChem workspace by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.
9. *Left click* on Display. *Left click* on Renderings. Choose sticks.
10. Repeat steps 1 and 2 of the Carbon Geometry section to start building CO<sub>2</sub>.
11. *Left-double click* again on the draw icon. The element table dialog box will again appear. *Left-double click* on Oxygen (O) in the periodic table. An Oxygen atom will appear. *Left click* to draw another Oxygen atom. Click and drag from Carbon to Oxygen twice to build two double bonds for CO<sub>2</sub>.
12. Repeat steps 4-7. Clear, following step 8.

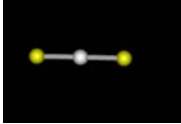
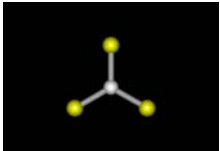
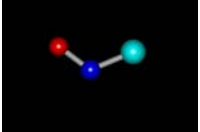
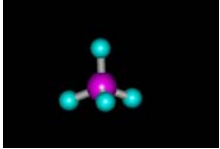

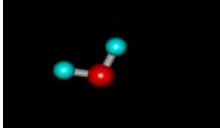
13. **To build molecules with a carbon chain:** *Left click* on Display. *Left click* on Renderings. Choose sticks. *Left click* Ok. *Left-double click* on the draw icon. The element table dialog box will appear. *Left-double click* on Carbon (C) in the periodic table.
14. *Left click* in the workspace. A Carbon atom will appear.
15. *Left click* in the workspace again to add more Carbon atoms to complete carbon chain. Add other non-hydrogen atoms (if molecule contains any) to the chain by: *Left-double clicking* on the draw icon. The element table dialog box will appear. *Left-double click* on non-hydrogen element in the periodic table. *Left click* in the workspace. The selected non-hydrogen atom will appear.
16. *Left click* on one carbon and drag to next, to build single bonds. Repeat to build a double bond between two carbons. Connect the non-hydrogen elements to carbon chain by *left clicking* on one carbon and dragging to the non-hydrogen element.
17. *Left click* Build. *Left click* on Add Hydrogens. A  $C_3H_6$  molecule will appear.
18. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK.  $C_3H_6$  molecule model is now complete and geometrically correct.
19. Measure bond angles for carbons following step 6.
20. Record angle measurements and clear the workspace, following steps 7 and 8.
21. **Build  $C_4H_8$ ,  $C_2H_6O$ ,  $HCOOH$ , and  $C_2H_5Cl$ , following these basic steps:**
  - a. Draw carbon chain (steps 12-14).
  - b. Add other elements except hydrogen (step 15).
  - c. Draw in bonds between carbon and non-hydrogen elements, omitting the hydrogen bonds. *Left click* -click on Add Hydrogen.
  - d. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK.
  - e. Measure bond angles for carbons following step 6. Record data and clear molecule.

### **Nitrogen Geometry**

1. *Left-double click* on drawing icon. *Left-double click* in Nitrogen (N). A Nitrogen atom will appear. *Left click* in workspace to draw another Nitrogen atom. Click and drag to connect Nitrogen atoms, three times forming a triple bond.
2. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. A  $N_2$  molecule model is now complete and geometrically correct.

3. Use different molecular rendering if desired at this time. *Left click* on Display. *Left click* on Renderings. Select type of rendering. *Left click* OK.
4. Clear N<sub>2</sub> molecule from the HyperChem workspace by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.
5. Repeat above steps as necessary to build NH<sub>3</sub> and CH<sub>3</sub>NH.
6. Measure the bond angle: For NH<sub>3</sub> and CH<sub>3</sub>NH<sub>2</sub> only.
  - a. *Left click* on Selection Tool.
  - b. *Left click* on one Hydrogen and drag cursor to another hydrogen. The bond angle will appear on the lower left below the workspace.
7. Record the bond angle, in degrees, on the Data Sheet.
8. Clear molecule from the HyperChem workspace by *left clicking* in an open area of the workspace. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule

Table 1 MOLECULAR STRUCTURES PREDICTED BY VSPER

Effective Pairs Around Central Atom	<u>Lone Pairs</u>	Shape, Angle and Hybridization	Bond Angle Example
2	0	Linear Example: BeF <sub>2</sub> Angle: 180 <i>sp</i>	
3	0	Triangular Planar Example: BF <sub>3</sub> Angle: 120 <i>sp</i> <sup>2</sup>	
3	1	Bent/Angular Example: ClNO Angle: 120 <i>sp</i> <sup>2</sup>	
4	0	Tetrahedral Example: CH <sub>4</sub> Angle: 109.5 <i>sp</i> <sup>3</sup>	
4	1	Triangular Pyramidal Example: NH <sub>3</sub> Angle: 106.7 <i>sp</i> <sup>3</sup>	
4	2	Bent Example: H <sub>2</sub> O Angle: 104.5 <i>sp</i> <sup>3</sup>	

**DATA SHEET**

Name \_\_\_\_\_

Name \_\_\_\_\_

Period \_\_\_\_\_ Class \_\_\_\_\_

Date \_\_\_\_\_

**POLARITY AND MOLECULAR SHAPE WITH HYPERCHEM LITE**

**DATA TABLE**

<b>Formula</b>	<b>Bond Angle Measurements</b>	<b>Shape</b>	<b>Non-Polar or Polar</b>
H <sub>2</sub> O			
CH <sub>4</sub>			
CO <sub>2</sub>			
C <sub>3</sub> H <sub>6</sub>			
C <sub>4</sub> H <sub>8</sub>			
C <sub>2</sub> H <sub>6</sub> O			
HCOOH			
C <sub>2</sub> H <sub>5</sub> Cl			
N <sub>2</sub>			
NH <sub>3</sub>			
CH <sub>3</sub> NH <sub>2</sub>			

## QUESTIONS

- How can molecular polarity be determined based on molecular shape?
- Although methane, water, and ammonia have similar molecular mass, their melting point and boiling points differ greatly. How does molecular shape and polarity of bonds affect boiling and melting points?

<b>Molecule</b>	<b>Boiling Point °C</b>	<b>Melting Point °C</b>
CH <sub>4</sub>	-161 <sup>0</sup>	-183 <sup>0</sup>
NH <sub>3</sub>	-33 <sup>0</sup>	-78 <sup>0</sup>
H <sub>2</sub> O	100 <sup>0</sup>	0 <sup>0</sup>