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 (\(\text{O}\)).
2. The element table dialog box will appear. **Left-double click** on Oxygen (O) in the periodic table.
4. **Left click** Build. **Left click** on Add Hydrogens. A \(\text{H}_2\text{O}\) molecule will appear.
5. Select Compute, **Left click** on Geometry Optimization. Select Polak-Ribiere. **Left click** OK. \(\text{H}_2\text{O}\) 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 H₂O 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**


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-H₄ bond, in degrees, on the data sheet.

8. Clear CH₄ 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.


10. Repeat steps 1 and 2 of the Carbon Geometry section to start building CO₂.


12. Repeat steps 4-7. Clear, following step 8.


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.


20. Record angle measurements and clear the workspace, following steps 7 and 8.

21. **Build C4H8, C2H6O, HCOOH, and C2H5Cl, following these basic steps:**
   a. Draw carbon chain (steps 12-14).
   b. Add other elements except hydrogen (step 15).
   e. Measure bond angles for carbons following step 6. Record data and clear molecule.

**Nitrogen Geometry**


2. Select Compute, *left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. A N2 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$_2$ 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$_3$ and CH$_3$NH$_2$.

6. **Measure the bond angle:** For NH$_3$ and CH$_3$NH$_2$ 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

<table>
<thead>
<tr>
<th>Effective Pairs Around Central Atom</th>
<th>Lone Pairs</th>
<th>Shape, Angle and Hybridization</th>
<th>Bond Angle Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>Linear</td>
<td><img src="image1.png" alt="Image" /></td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>Triangular Planar</td>
<td><img src="image2.png" alt="Image" /></td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>Bent/Angular</td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>Tetrahedral</td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>Triangular Pyramidal</td>
<td><img src="image5.png" alt="Image" /></td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>Bent</td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
</tbody>
</table>
DATA TABLE

<table>
<thead>
<tr>
<th>Formula</th>
<th>Bond Angle Measurements</th>
<th>Shape</th>
<th>Non-Polar or Polar</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₄</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO₂</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₃H₆</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₄H₈</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₂H₆O</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HCOOH</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₂H₅Cl</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N₂</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH₃</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃NH₂</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
QUESTIONS

1. How can molecular polarity be determined based on molecular shape?

2. 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?

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Boiling Point °C</th>
<th>Melting Point °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>-161⁰</td>
<td>-183⁰</td>
</tr>
<tr>
<td>NH₃</td>
<td>-33⁰</td>
<td>-78⁰</td>
</tr>
<tr>
<td>H₂O</td>
<td>100⁰</td>
<td>0⁰</td>
</tr>
</tbody>
</table>