MOLECULAR MODELING AND GEOMETRY WITH HYPERCHEM LITE

LAB MOD 5.COMP
From Gannon University SIM

INTRODUCTION

The properties of molecules depend upon bonding. Equally important is the arrangement of the atoms in space, molecular geometry. Two theories used to explain the molecular geometry observed for molecules are **VSEPR** and **Hybridization**. Both of these theories can also be used to predict the molecular geometry of molecules for which the shape is unknown.

The VSEPR theory for predicting molecular geometry is 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.

Hybridization is the second theory for predicting molecular geometry. It is a more sophisticated refinement of VSEPR that successfully explains the molecular geometries of more complex molecules. Hybridization is the mixing of two or more atomic orbital of similar energies on the same atom to give new orbitals of equal energies. The type of hybridization of the central atom and non-bonded electron pairs affects the geometry of a molecule.

PURPOSE

The purpose of this experiment is to learn to measure bond angles and study the shape and geometry of molecules and the effect of unshared pairs of electrons on bond angles, 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. <u>Menu Bar</u>: contains the different HyperChem Lite menus which include: File, Edit, Build, Display, Set-up, Compute, Cancel and Help.

   b. <u>Tool Bar</u>: the left side of the screen contains the tools to draw, select, display and move atoms and molecules.

   c. <u>Workspace</u>: displays current atoms or molecules.

   d. <u>Status Line</u>: show a brief description of menu item selected and information about drawing.

   e. <u>Title Bar</u>: shows name of file working on.

   f. <u>Control Menu Button</u>: contains commands to move, resize, maximize, and close HyperChem Lite windows. It also contains the switch command, which lets you activate other windows.

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_4 molecule will appear.

4. Select Compute, *Left click* on Geometry Optimization. Select Polak-Ribiere. *Left click* OK. CH_4 molecule model is now complete and geometrically correct.

5. Use ball and cylinder molecular rendering at this time. *Left click* on Display. *Left click* on Renderings. Select ball and cylinder, shaded and highlighted. *Left click* OK.

6. <u>Measure the bond angle</u>:
   a. *Left click* on Selection Tool.
   b. *Left click* on one hydrogen and drag cursor across the carbon atom to another hydrogen. The bond angle will appear on the lower left below the workspace.

7. Record bond angle, in degrees, for the $C-H_4$ bond on Data Sheet.

8. Clear CH_4 molecule from the HyperChem workspace by *left clicking* in an open area of the workspace with the selection tool. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.

Nitrogen Geometry

1. *Left-double click* on drawing icon (⊕).*Left-double click* in Nitrogen (N); repeat steps 3-5 as above in the Carbon Geometry section.

2. <u>Measure the bond angle</u>:
   a. *Left click* on Selection Tool.
   b. *Left click* on one Hydrogen and drag cursor across Nitrogen atom to another hydrogen. The bond angle will appear on the lower left below the workspace.

3. Record bond angle, in degrees, for the bond on Data Sheet.

4. Clear NH_3 molecule from the HyperChem workspace by *left clicking* in an open area of the workspace with the selection tool. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.

Oxygen Geometry

1. *Left-double click* on drawing icon (⊕).*Left-double click* in Oxygen (O); repeat steps 3-5 as above in the Carbon Geometry section.

2. <u>Measure the bond angle</u>:
   a. *Left click* on Selection Tool.
   b. *Left click* on Hydrogen and drag cursor to other Hydrogen. The bond angle will appear on the lower left below the workspace.

5. Record bond angle, in degrees, for the bond on Data Sheet.

3. Clear H_2O molecule from the HyperChem workspace by *left clicking* in an open area of the workspace with the selection tool. All the atoms will turn green. Select Edit and *left click* on clear. Select yes to remove the previous molecule.

DATA SHEET

Name _____

Name _____

Period _____ Class _____

Date   _____

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DATA TABLE

Molecule	Bond Angle Measurement (deg.)
CH_4	
NH_3	
H_2O	

QUESTIONS

1.   Draw the three-dimensional structure of CH_4. What type of hybridization does the carbon have?

2.   Draw the three-dimensional structure of NH_3. Put in the non-bonded pair of electrons. What effect did the non-bonded pair have on the bond angles to the hydrogens?

3.   Draw the three-dimensional structure of H_2O. Put in your drawing the two non-bonded electron pairs. What effect did the two non-bonded pairs have upon the bond angles to hydrogen?