

HyperChem Lite: Molecular Modeling and Geometry

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.

Introduction:

The properties of molecules depend upon bonding. Equally important is the arrangement of the atoms in space or molecular geometry. There are two theories to predicting molecular geometry: VSEPR and Hybridization.

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 predicting molecular geometry. **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.

Guiding Question:

Please answer the following question before completing the experiment.

When determining the shape a certain molecule will take, the number of bonds around the central atom must be considered. What else around the central atom must be considered when determining molecular shape?

Equipment/Materials:

- Computer with HyperChem Lite software program installed
- Mouse (optional)
- Mouse pad (optional)

Procedure:

1. Left (L)-double click on the Draw Icon at the top left of the screen (Figure 1). The Element Table dialog box will appear. (L)-double-click (DC) on beryllium on the periodic table.
2. L-click in the workspace to place a beryllium atom on the screen.



Figure 1:
Draw Icon

3. L-click Build. L-click on Add H & Model Build. A complete molecule will appear. (Don't freak out! Your molecule should indeed look like a line at this point. Just keep going – it gets better!)
4. 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.
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 model is now complete and geometrically correct. **Note: Geometry Optimization must be done for every molecule built!**
7. To rotate the molecule in the X and Y planes, first L-click on the XY Rotation Tool (Figure 2). Next, L-click and drag in the workspace to rotate the molecule in any direction.
8. To rotate the molecule in the Z plane, L-click on the Z Rotation Tool (Figure 3). Next, L-click and drag in the workspace.
9. To measure the bond angle:
 - a. L-click on Selection Tool (Figure 4).
 - b. L-click at the center of one hydrogen and drag the cursor across to the center of the other hydrogen. The bond angle will appear on the lower left below the workspace.
10. In the data section, record the bond angle, the shape of the molecule, and they hybridization of the central atom.
10. 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 4). L-click in workspace outside of the molecule; the molecule will turn green. L-click Edit, L-click clear, and then answer Yes.
11. Repeat the above procedure to complete the data table. For the last two, make sure that allow ions is checked in the build menu. For PH₅, there are 3 different bond angles. For SF₆, there are 2 bond angles; to build it, manually place all



Figure 2: XY
Rotation Tool



Figure 3: Z
Rotation Tool



Figure 4:
Selection Tool

atoms on the screen, and then connect them by clicking at the center of one atom and dragging to the center of another. You MUST still click on Add H & Model Build to get the correct shape!!

Data:

Molecule	Bond Angle (°)	Shape	Hybridization
BeH ₂			
BH ₃			
H ₂ O			
NH ₃			
CH ₄			
PH ₅			
SF ₆			

Questions:

1. What effect do non-bonding electron pairs have on molecular shape?

2. Identify the following molecules as polar or non-polar.

a. BeH_2

b. BH_3

c. H_2O

d. NH_3

e. CH_4

f. PH_5

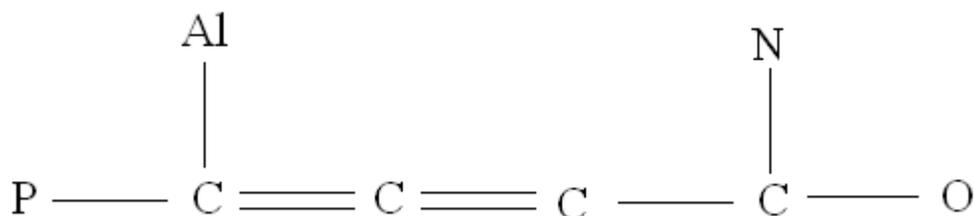
g. SF_6

Extension 1 (optional):

Use HyperChem Lite to build other molecules from your text. Measure their bond angles and determine their shapes and hybridizations. Create a data table to record your data.

Extension 2 (optional): An Organic Molecule**Procedure:**

1. Recreate the image below. (Be sure to draw the double bonds as shown.)



2. L-click Build. L-click on Add H & Model Build.
3. If the molecule has changed its orientation on the screen, rotate it until the carbon atom that is bonded to the phosphorus and aluminum atoms is on the left and the carbon atom that is bonded to the nitrogen and oxygen atoms is on the right, as above. Use the rotation tools if needed. (Figures 2 & 3.)
4. For data collection, the carbons will be identified as follows:
 - Carbon 1: bonded to the phosphorus and aluminum atoms
 - Carbon 2: double-bonded to two other carbons
 - Carbon 3: double-bonded a carbon atom and single-bonded to another
 - Carbon 4: bonded to the nitrogen and oxygen atom

(Note: if the molecule is correctly oriented on the screen, these carbons will be in order from left to right.)

5. Complete the data table, looking at the structure around each atom listed, not the molecule as a whole. Rotate the molecule as needed to see the structure. There will be slight variations in the bond angles due to the different pulling or pushing abilities of different bonds. Approximate.

Data:

Molecule	Bond Angle (°)	Shape	Hybridization
C ₁			
C ₂			
C ₃			
C ₄			
P			
Al			
N			
O			