What Are the Shapes of Molecules?

Pre-Lab Assignment

Read the entire lab handout. There is no written pre-lab assignment for this lab.

Learning Goals

- Derive the Lewis structure of a covalent molecule from its model.
- Draw 3-dimensional shapes on paper using the wedge and dash convention.
- Classify molecular shapes according to the VSEPR model.
- Describe how the chemical bonding possibilities for carbon lead to a diversity of structure in carbon compounds.
- Explain the implications of the left- and right-handed nature of chiral compounds.

Background

Covalent bonds are formed between atoms of nonmetallic elements. A covalent bond consists of a pair of electrons shared by the bonded atoms. The octet rule states that an atom is chemically stable if eight valence electrons are present around the nucleus. The eight valence electrons are arranged in four pairs, which results in different bonding character for each representative group.

- Group IVA atoms can have four single covalent bonds. Example: CH₄
- Group VA atoms usually have three single covalent bonds. The fourth pair in the octet does not bond and is called a “nonbonding electron pair.” Example: NH₃
- Group VIA atoms usually have two covalent bonds and two nonbonding electron pairs. Example: H₂O
- Group VIIA atoms usually form one covalent bond and have three nonbonding electron pairs. Example: Br₂

The shapes, or geometry, of single bonded molecules are derived from the Valence Shell Electron Pair Repulsion model, aka the VSEPR theory. According to this theory, the four electron pairs must repel each other and find positions that are as far apart as possible. The result is that the shape of the molecule can be predicted if the number of bonding and nonbonding electrons are known. For octet systems, the following table works well for molecules with only single bonds.

<table>
<thead>
<tr>
<th>Group</th>
<th>Example</th>
<th>Bonding e⁻ Pairs</th>
<th>Nonbonding e⁻ Pairs</th>
<th>Total e⁻ Pairs (electron domains)</th>
<th>VSEPR Geometry</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIA</td>
<td>BH₃</td>
<td>3</td>
<td>0</td>
<td>3</td>
<td>Trigonal Planar</td>
<td></td>
</tr>
<tr>
<td>IVA</td>
<td>CCl₄</td>
<td>4</td>
<td>0</td>
<td>4</td>
<td>Tetrahedral</td>
<td></td>
</tr>
<tr>
<td>VA</td>
<td>NH₃</td>
<td>3</td>
<td>1</td>
<td>4</td>
<td>Trigonal Pyramid</td>
<td></td>
</tr>
<tr>
<td>VIA</td>
<td>H₂O</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>Bent or Angular</td>
<td></td>
</tr>
<tr>
<td>VIIA</td>
<td>Br₂</td>
<td>1</td>
<td>3</td>
<td>4</td>
<td>Linear</td>
<td></td>
</tr>
</tbody>
</table>
Many compounds do not follow the octet rule. Two examples are arsenic pentafluoride and sulfur hexafluoride.

<table>
<thead>
<tr>
<th>Example</th>
<th>Bonding e⁻ Pairs</th>
<th>Nonbonding e⁻ Pairs</th>
<th>Total e⁻ Pairs</th>
<th>VSEPR Geometry</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>AsF₅</td>
<td>5</td>
<td>0</td>
<td>5</td>
<td>Trigonal Bipyramidal</td>
<td>![Trigonal Bipyramidal Structure]</td>
</tr>
<tr>
<td>SF₆</td>
<td>6</td>
<td>0</td>
<td>6</td>
<td>Octahedral</td>
<td>![Octahedral Structure]</td>
</tr>
</tbody>
</table>

Many elements may form multiple bonds between atoms. Carbon is an important example of an element that can form double and triple covalent bonds to satisfy the octet rule. The presence of double or triple bonds will affect the shape classification of the carbon atom in the compound. For example, a carbon atom with one double bond and two single bonds will have three electron domains (areas of electron density) and will form a trigonal planar geometry, similar to a group IIIA element. Carbon atoms with two double bonds, or one triple bond plus one single bond will have two electron domains and will form a linear geometry, similar to a group IIA element.

Since carbon has the ability to form tetrahedral, trigonal planar, and linear shapes within any given molecule, carbon compounds have tremendous diversity and potential complexity in molecular structure since a single molecule may contain many carbon atoms. This is the direct cause of the variety of sugars, proteins, DNA and other molecules which are the basis of the many life forms found on Earth.

**Drawing 3-D Structures**
- Atoms in a plane are connected with solid lines.
- An atom pointed toward you is connected with a wedged line.
- An atom pointed away is connected with a dashed line.

**Table of Wedge-and-Dash Geometries**

<table>
<thead>
<tr>
<th>Number of Electron Domains</th>
<th>Arrangement of domains for maximum separation Electron Domain Geometry = Parent Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>![2 Electron Domains Geometry]</td>
</tr>
<tr>
<td>3</td>
<td>![3 Electron Domains Geometry - Top View]</td>
</tr>
<tr>
<td>4</td>
<td>![4 Electron Domains Geometry]</td>
</tr>
</tbody>
</table>
Lab 7: What are the Shapes of Molecules?

**Procedure**

My lab partner is: ________________________________

Obtain a model kit. Note that in most cases the following color convention is used.

- Carbon - black, 4 holes
- Nitrogen - blue, 4 holes
- Hydrogen - white, 1 hole
- Oxygen - red, 2 holes
- Halogens 1 hole: Fluorine - Orange
- Chlorine - Green
- Bromine - Brown
- Iodine - Purple

The atoms are predrilled with the proper number of holes at the correct angles to represent the bonding capabilities of the individual elements. Notice that in the case of oxygen and all halogens, holes for nonbonding electron pairs are not present.

1. **Build the model first.**
   - For each of the compounds in parts A to D, construct the molecular model using the pre-drilled holes as a guide for bonding the atoms together. You should be able to account for an octet of electrons around each atom in the molecule (except hydrogen, which needs only 2 electrons).

2. **Draw a 3-D sketch while looking at the model.**
   - Use the wedge and dash convention to draw a 3-D sketch of the model. Add nonbonding electron pairs where needed for the atoms to have an octet of electrons.

3. **Get instructor initials for each model/drawing.**
   - Before disassembling the molecules, have the models and your wedge-and-dash sketch approved by the instructor, who will initial each entry in your lab report.

Please use a pencil to complete this handout.

**Part A: Tetrahedral-based Shapes of Groups IVA, VA, and VIA**

Notice that the four electron pairs around any atom occupying a central position between two or more other atoms are oriented in the tetrahedral shape. **When nonbonding electrons are present, such as in NH₃, the name of the shape changes to trigonal pyramidal, but the four pairs still have the tetrahedral orientation.**

1. Methane: CH₄
2. Ammonia: NH₃

3. Ethanol: CH₃CH₂OH
4. Water
**Part B: Multiple Bonds of Carbon**

Use the longer, flexible connectors to represent the multiple bonds. A double bond is two electron pairs and requires two connectors. A triple bond requires three connectors.

Carbon is an extremely versatile element. In the following compounds look for multiple bonds at the carbon atom and note how the geometry is no longer tetrahedral.

5. Formaldehyde: $\text{H}_2\text{C}=\text{O}$
6. Carbon Dioxide
7. Acetylene: $\text{HCCH}$

8. Benzene: $\text{C}_6\text{H}_6$
   Hint: The six carbon atoms are in a ring with alternating single and double bonds.

9. Aspirin: $\text{C}_9\text{H}_8\text{O}_4$
   Use the benzene molecule as the basis for this molecule. The instructor will draw the full structure on the board.

---

**Part C: Isomers**

Molecules with the same formulas may have structural differences that cause them to be different compounds. Compounds with the same molecular formula but different structures (atoms connected differently) are called structural isomers.

10, 11, and 12. Dichloroethylene: $\text{C}_2\text{H}_2\text{Cl}_2$

This model can be made three different ways. Construct all three molecules. Demonstrate that the double bond will not allow the carbons to rotate. This locks the four attached atoms into fixed configurations. Hint: The carbons are double-bonded to each other in each molecule.
Data Analysis and Exercises

Complete these questions on a separate sheet of paper.

1. Construct a table with the following column headings: Molecular Formula, Lewis Structure, 3-D Drawing, Molecular Shape. Your table will have 14 data rows – one for each compound in this lab. Neatly fill in the table. Note that for Molecular Shape, you will need to name the shape around each central atom when there is more than one central atom.
   
   Hint: To confirm that you have drawn the correct Lewis structures, be sure to check (1) that you have the correct total number of valence electrons for the molecule and (2) that each atom in the molecule has an octet.

2. Classify the shapes of the following molecules. Show all work.
   a. PCl₃  
   b. SO₂  
   c. SBr₂  
   d. SiH₄  
   e. CS₂

3. Describe how the chemical bonding possibilities for carbon lead to a diversity of structure in carbon compounds.

4. Extra Credit: The following structures do not necessarily follow the octet rule. Name the shapes of the following molecules. Show all work.
   a. PCl₅  
   b. H₃O⁺  
   c. XeF₂  
   d. SF₆  
   e. NO₃⁻

Lab Report

The lab report includes the following stapled in order:

1. This handout.
2. Data Analysis and Exercises written on a separate sheet.