LAB 11 – Molecular Geometry

Objectives

At the end of this activity you should be able to:

- Write Lewis structures for molecules.
- Classify bonds as nonpolar covalent, polar covalent, or ionic based on electronegativity differences.
- Recognize exceptions to the octet rule; draw accurate representations.
- Describe 3-dimensional shapes of simple molecules based on VSEPR theory.
- Predict polarity based on geometry and individual dipole moments.

To complete this lab, you will use a handout obtained from:
http://www.sci.uidaho.edu/chem101/Lecture-supplements/VSEPR1.PDF
and you will use an online computer simulation found at:
https://phet.colorado.edu/en/simulation/molecule-shapes

Submit all of your completed tables to your lab instructor by Friday at 3 pm for grading.

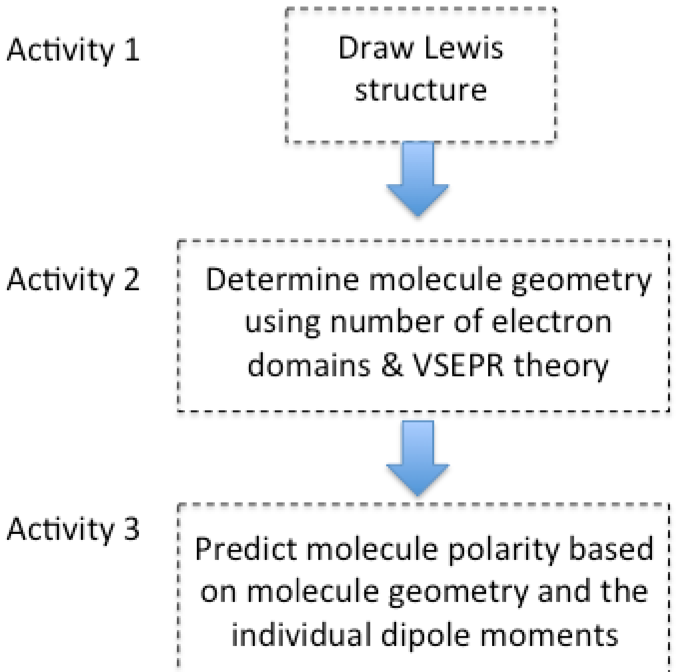
Introduction

The substances in our world exhibit remarkably different properties. At room temperature some substances are solids, others liquids, and others gases. Some participate in sudden chemical reactions, whereas others are quite inert and unreactive. Perhaps most remarkably, this wonderful diversity occurs even though the substances are comprised of a limited number of elements. Indeed, only a very small number of different elements are present in almost any pure substance we encounter in the environment or the laboratory. How can this wide diversity of properties be explained?

A key to understanding the wide range of physical and chemical properties of substances is recognizing that atoms *combine* with other atoms to form molecules or compounds and that the *shape or geometry* of a collection of atoms strongly affects the properties of that substance. One reason this occurs is because the distribution of charge in a molecule affects many properties of the substance. For example, if the negative charge is concentrated in one region of a molecule its properties will be widely different than if the charge is distributed evenly throughout the entire molecule. In this investigation you will examine a theory that chemists use to explain different aspects of chemical bonding: *Valence-shell electron-pair repulsion* (VSEPR) theory. Attention will be given to how molecules are arranged in different shapes and how chemists can predict the geometry of a given molecule. It will then be shown how a molecule's shape, along with electronegativity differences for atoms, determines the molecule's polarity. As suggested above, the best way to understand and predict the physical and chemical properties of substances in our world is by understanding their structure at the molecular level.

Discussion of Activities

In this investigation you will complete activities that ask you to examine molecular geometry and molecular polarity. These activities are based on computer simulations and ball-and-stick models. All of these activities can be discussed with classmates and/or completed in small groups. The VSEPR model can be used to predict the geometry of molecules and polyatomic ions. *Molecular geometry* describes the positions of the nuclei in relation to each other. Included in the description are the *bond angles*, the angles made by the lines joining the nuclei of bonded atoms. In order to predict geometry using the VSEPR model, we need to know the number of electron pairs in the valence shell of the central atom. That can easily be determined by drawing a Lewis structure.



Activity 1: Drawing Lewis Structures

Table 1. Drawing Lewis Structures and Determining Electron & Bonding Domains.

	Sketch of Lewis structure	Does the structure violate the octet rule"?	Number of electron domains (central atom)	Number of bonding domains (central atom)
NH_3				
H_2O				
BF_3				
CO_2				
XeF_6				

Activity 2: VSEPR and Predicting Molecular Geometry

Once we have the Lewis structure, we have the information needed to predict the geometry. It's important to remember that what we really want to know is the *molecular geometry*—the positions of the nuclei in relation to each other. The molecular geometry is dependent on the electron domain geometry; that is why the initial step is drawing the appropriate Lewis structure! As noted above, the simple concept behind valence shell electron pair repulsion theory (VSEPR) is the idea that electron pairs in the valence shell of an atom will repel each other and arrange themselves as far apart as possible. This arrangement of electron pairs will determine the geometry of the molecule or polyatomic ion. To help you make predictions, use the VSEPR handout and the PHET simulation. You may also search the web for structures. You will be given the handout on your final exam.

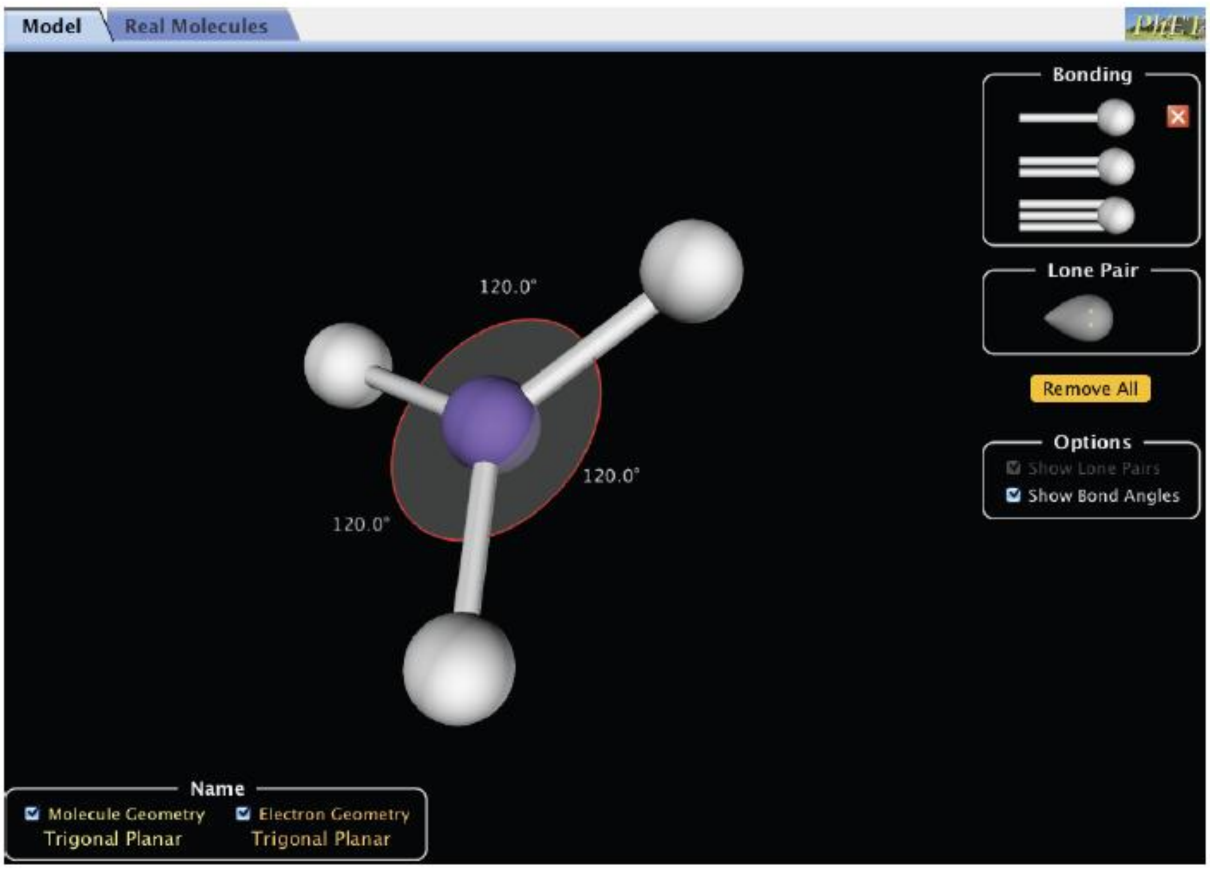


Figure 1. The PhET Computer Simulation "Molecule Shapes".

Your initial task in this activity is to determine the molecule geometry as the number of electron pairs changes. Accomplish this by using **the computer simulation "Molecule Shapes"** (shown above) (https://phet.colorado.edu/en/simulation/molecule-shapes) and the VSEPR handout (**http://www.sci.uidaho.edu/chem101/Lecture-supplements/VSEPR1.PDF**) and fill in the table. Notice, in this simulation you can increase the number of electron domains by adding single, double, or triple bonds, or lone pair electrons. In the lower left corner you will find both the molecule geometry and the electron geometry.

Table 2. Model Electron Domain Geometries.

Number of Electron Domains	Electron Domain Geometry	Bond Angles
2	Linear	180°
3		
4		
5		
6		

The molecular geometry is the same as the electron domain geometry **if** all domains contain bonding pairs. What if lone pair electrons are present on the central atom? The molecular geometry will **NOT** be the same as the electron domain geometry. To investigate this, return to the simulation and complete Table 3. If you do not understand the names for the different geometries consult the handout.

Table 3. Electron and Molecular Geometries.

Number of electron domains	Bonding Pairs	Nonbonding Pairs	Electron Domain Geometry	Molecular Geometry
2	2	0		
3	3	0		
3	2	1		
4	4	0		
4	3	1		
4	2	2		
5	5	0		
5	4	1		
5	3	2		
5	2	3		
6	6	0		
6	5	1		
6	4	2		

In the last table, you are asked also to determine molecule polarity. Read or review section 9-9 and the Summary Chart on page 309 of your textbook.

Putting it all together…

Being able to predict the polarity of a molecule is extremely important since many properties of molecules depend on whether they are polar or non-polar. As you have seen in this activity, determining a molecule's polarity is a multi-step process:

Draw Lewis Structure

↓

Use VSEPR to determine molecular geometry

↓

Determine bond polarity (based on electronegativity differences)

↓

Determine molecular polarity based on bond dipoles & molecular geometry

For the following molecules complete this step-by-step process.

Molecule	Lewis Structure	Molecular Geometry	Is there a molecular dipole? A molecular dipole indicates it is a polar molecule.
N_2			
H_2O			
BF_3			
HCN			
CH_2F_2			

* Make a prediction, and then check it in the "Real Molecules" section of the simulation.