Introduction

This exercise provides procedures to determine the structure and shape of molecules. This information is important because the properties of molecules are dependent upon their structure. The first step in determining the structure (Lewis structure) of a molecule is to draw a structure accurately showing the location of all valence electrons. From the Lewis structure, you can use a method called valence shell electron pair repulsion (VSEPR) theory to predict the shape of a molecule or ion.

In order to use VSEPR, you need to be able to determine the number of electron groups bonded to the central atom and the number of atoms bonded to the central atom. Lastly, after you have determined the molecule's shape, you can determine whether electron density in the molecule is arranged symmetrically (a nonpolar molecule) or asymmetrically (a polar molecule). In a polar molecule, one end of the molecule has a partial positive charge, one end has a partial negative charge. The polarity of a molecule has important implications for the properties of molecules.

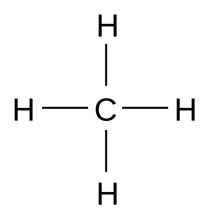
Theory of VSEPR

In order to use VSEPR, it is necessary to have a completed Lewis structure for the molecule. VSEPR is based on the principle that electron groups in a molecule tend to stay as far apart from each other as possible due to the repulsive forces that exist between like charges (the electrons). An electron group could be a lone pair of electrons, a single bond, a double bond or a triple bond around the central atom. The most probable arrangement of two, three, or four electron groups around a central atom are given in the table below. This arrangement allows groups to spread out as far as possible.

Table 1. Electron Group Geometries

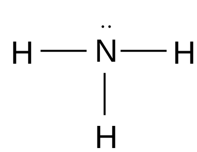
# of Electron Groups	**Electron Group Geometry**
2	Linear
3	trigonal planar
4	Tetrahedral

As an example, let's consider methane, CH_4. The Lewis structure for methane is given below:



In this case we can see that there are four electron groups (4 single bonds) surrounding the carbon atom, hence the geometric arrangement of the electrons about the carbon atom is tetrahedral.

Ammonia, NH_3, is a little more difficult.



The Lewis structure for ammonia shows that there are four electron groups (3 single bonds and 1 lone pair of electrons) therefore the electron group geometry is also tetrahedral. It should be noted however that CH_4 has 0 lone pair electrons, while NH_3 only has 1 set of lone pair electrons bonded to the central atom. Ammonia therefore they will not have the same shape as CH_4. Molecular shape describes the arrangement of **atoms** about the central atom.

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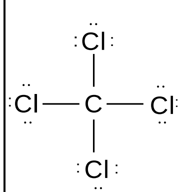
When determining the molecular shape, you must consider the electron group geometry and the number of **lone pairs** bonded to the central atom. The possible combinations of electron groups and lone pair electrons are summarized in the chart I gave you.

Using our chart, we can predict that CH_4 has a tetrahedral molecular shape while NH_3 has a trigonal pyramidal molecular shape.

After the geometries have been assigned to a molecule, we decide if there is more than one correct structure for it. These correct structures are called resonance structures. Lastly, we can use the molecular shape to determine if electron density is evenly distributed across the molecule. If electron density is unevenly distributed across the molecule, the molecule is said to be polar. A molecule with a uniform charge distribution is nonpolar. But first you must learn how to draw Lewis dot structures…

The Assignment

You are to determine the Lewis structure, electron pair geometry, molecular geometry, expected bond angle and the polarity for a series of molecules given on the worksheet. Feel free to work on this exercise in a group to help you learn the procedure. Carbon tetrachloride is worked out for you as an example.

	CCl_4	BF_3	SO_3	CO_2
Lewis Structure				
Resonance structures (if any)				
Molecular Geometry	tetrahedral			
Expected Bond Angle	109.5			
Polar or nonpolar	Nonpolar			
IMFs present	LDF			

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Names: ______________________________________ Date: ___________

	H_2O	SO_4^{2-}	NO_2^+	PO_4^{3-}
Lewis Structure				
Resonance structures (if any)				
Molecular Geometry				
Expected Bond Angle				
Polar or nonpolar				
IMFs present				

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	CO_3^{2-}	SO_2	NO_2^-	PF_3	
Lewis Structure					
Resonance structures (if any)					
Molecular Geometry					
Expected Bond Angle					
Polar or nonpolar					
IMFs present					

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	NH_3	H_3O^+	NH_4^+	SO_3^{2-}
Lewis Structure				
Resonance structures (if any)				
Molecular Geometry				
Expected Bond Angle				
Polar or nonpolar				
IMFs present				

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	SiI_4	$CHCl_3$	NO_3^-	ClO_2^-	
Lewis Structure					
Resonance structures (if any)					
Molecular Geometry					
Expected Bond Angle					
Polar or nonpolar					
IMFs present					