EXPERIMENT 15:
MOLECULAR MODELS

Introduction: Given formulas of some molecules and ions, you will use the periodic table, valence electron count, and electronegativities to deduce their geometry and polarities.

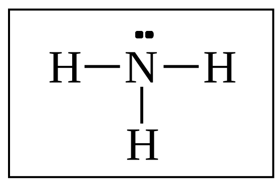
Background: Around 1916, G. N. Lewis proposed that a bond in a molecule consisted of an electron pair. Guidelines for drawing covalent bonds were formulated. These guidelines can be applied best to molecules and ions formed by the non-metals of the representative elements (specifically hydrogen) and groups 14-17 (4A-7A).

The most critical aspect in determining structures according to Lewis theory is the octet rule. All atoms in the correct structure will have eight electrons (the octet) surrounding them. These electrons may be present as either pairs in bonds or as non-bonded pairs. The exception is the element hydrogen, which will have a duet, or two electrons. The s and p valence orbitals are filled and their total capacity is eight electrons
(s^2p^6 configuration) A valence octet is particularly stable. Thus, one has the **octet rule.**

In addition, the **electronegativity** of the bonded atoms determines whether the electrons are evenly distributed in the molecule. Electronegativity represents an atom's ability to attract the electrons in a bond. F is the most electronegative.

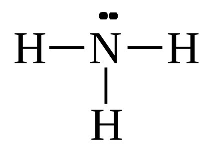
Element	Electroneg.	Element	Electroneg.	Element	Electroneg.	Element	Electroneg.
H	2.1	B	2.0	C	2.5	N	3.0
O	3.5	F	4.0	Si	1.8	P	2.1
S	2.5	Cl	3.0	Br	2.8	I	2.5

An example of a Lewis structure is that for ammonia, NH_3.
Note that a line (—) is used to represent a two-electron bond and a pair of dots (:) is used to represent a non-bonded electron pair (also called a "lone pair"). The Lewis structure of ammonia is shown:



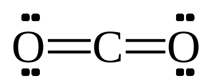
This structure conforms to the octet rule. Each hydrogen has one bond (two electrons), and the nitrogen is surrounded by three bonds and one non-bonded pair (a total of eight electrons). There is a set of steps to follow in determining this structure:

Steps	NH_3 Example
1. Determine the total number of valence electrons in the molecule. The number of valence electrons for an element is equal to the second digit of the group number. Groups 14-17 have four to seven valence electrons, respectively.	N is in group15 and has five valence electrons. H is in group1 and has one valence electron. 5 + 3x1 = **8 valence electrons** If a formula has a – charge, add an electron or electrons. A few formulas have + charge so subtract an electron.
2. Set up a "skeleton" arrangement with the central atom in the middle, boxed in by the outer atoms	N is central, surrounded by 3 H's.
3. Draw the minimum number of bonds	Draw 3 x N-H bonds. This represents 6

necessary to hold the molecule together.	Electrons.
4. Subtract the (# bonds x2) from the total # of valence electrons. Distribute the remainder as pairs.	**8 – (3 bonds x2) = 2 (2 e^- = 1 lone pair)**
5. Calculate the number of remaining electrons after all bonds have been formed and distribute them to complete the octet requirement of each atom. (H is satisfied with 2.)	N lacks an octet and has only 6 electrons. Place the remaining 2 electrons as a non-bonded pair on N. 

Not all molecules will have only single bonds as in NH_3 above. Double bonds (=) and triple bonds (≡) are possible. **Consider carbon dioxide, CO_2.** Follow the steps above:

1. C= 4 valence electrons; O= 6 valence electrons   4 + (2 x 6) = **16 electrons** available
2. Arrange atoms: O C O
3. Place minimum of 2 bonds, O – C – O
4,5. Electrons that remain are 16 – 8 = **8.** Since the atoms lack an octet, distribute the remaining 8 electrons as additional bonds or lone pairs so all atoms obey the **octet rule.**

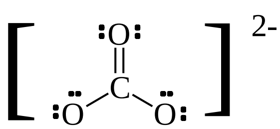


Finally, with an ion, you must add the number of electrons equal to the negative charge of an anion; or subtract a number of electrons equal to the positive charge of a cation. Consider CO_3^{2-}**:**

1. 4 + 3 x 6 + **2** (negative charge) = 24 electrons
2,3. Arrange the 4 atoms and draw three bonds.

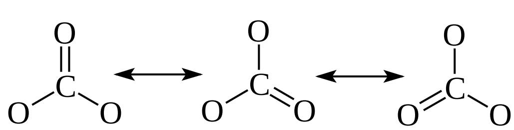
O - C - O
    |
    O

4,5 24 – 6 = 18 Arrange these 18 electrons as pairs or additional bonds

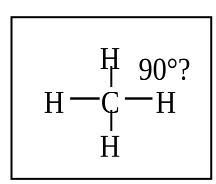
7. 

Note that brackets are drawn and the charge indicated

The structure of CO_3^{2-} could have been drawn in three different ways:

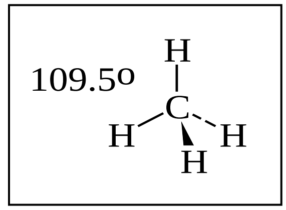


All are equally valid "resonance structures." The arrow, ↔, is used to show "resonance" or "electron delocalization." The correct structure is an average of all of the resonance structures. We will not concern ourselves with this in this experiment.



VSEPR structures: Lewis structures are generally drawn flat. However, the arrangement of atoms in a molecule is not necessarily flat. A simple example is CH_4: Each bond and non-bonded electron pair represents a region of electron density. Electrons repel each other to move as far apart as possible to minimize repulsion

The Lewis structure may not show the actual three-dimensional structure of the molecule when electron repulsion is considered. When this repulsion is taken into account, we use the <u>V</u>alence <u>S</u>hell <u>E</u>lectron <u>P</u>air <u>R</u>epulsion method (VSEPR). Minimum repulsion in CH_4 occurs if the molecule takes on a geometry called tetrahedral, as shown here.

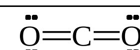
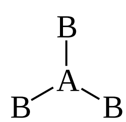
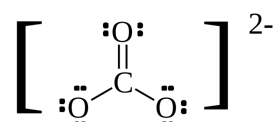
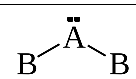
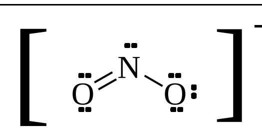
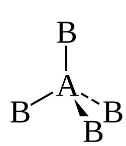
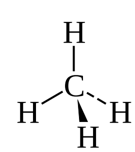
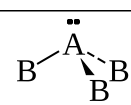
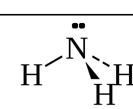
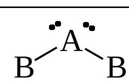
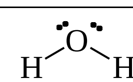


Notice that the bond angle has increased from 90 to 109.5^o, minimizing repulsion. A convention for drawing bonds in 3-D space, is as follows:

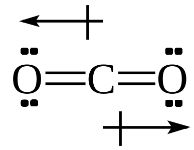
The wedge,	▬	represents a bond coming out of the paper
The dash,	-----	represents a bond going behind the paper
The line,	——	represents a bond on the paper

Examine a model of CH_4 from the model kit so that you can relate the type of bonds drawn to the three-dimensional arrangement.

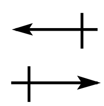
Fortunately, the VSEPR structure can be drawn directly from the Lewis structure. The determining factor in the VSEPR structure is the **number of regions of electron density around the central atom**. A region of electron density will be either a non-bonded electron pair or a bond. For VSEPR purposes, <u>it does not matter whether the bond is single, double, or triple.</u> We count only lone pairs & bonds on the central atom
Using the designation of "A" for the central atom, "B" for any atoms or groups that are bonded to the central atom, and "E" for a non-bonded electron pair, molecules and ions can be classified as follows according to their VSEPR structures:

Regions of electron density	**Possible electron & atom arrangements**	**Molecular structure, approx. bond angles**	**Example**
2	AB_2, B—A—B	Linear 180^o	
3	AB_3, 	Trigonal planar 120^o	
3	AB_2E, 	Bent or angular 120^o	
4	AB_4, 	Tetrahedral 109.5^o	
4	AB_3E, 	Trigonal pyramidal 109.5^o	
4	AB_2E_2, 	Bent or angular 109.5^o	

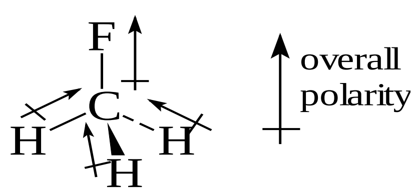
Polarities of bonds and molecules: The last aspect of a molecule or ion's properties that can be determined is the polarity of the bonds and the overall polarity of the species. Any bond must be polar if the electronegativities of the atoms are different. The electrons will be more attracted to the more electronegative atom causing this atom to be partially negative and the other atom to be partially positive. However, the molecule overall may not be polar. Consider the following examples:



Arrows are used to indicate bond polarity. The arrowhead points toward the more electronegative atom (oxygen) and the cross is near the less electronegative atom (carbon). These arrows can actually be moved around as long as their direction is not changed. In fact, they can be moved so that they are directly below each other.



The arrows are of equal length, but in opposite directions, and cancel. Whenever the polarities of bonds cancel in this way, the molecule is non-polar. You can imagine the bond polarities being centered in the center of the molecule. When this is the case, they will cancel. A good example is CH_4. Although it is tetrahedral, the polarities still center at the center of the molecule and cancel. However, consider a related molecule, CH_3F. This is drawn below with the polarity arrows:



Notice that all of the polarity arrows point in a general upward direction leading to the overall molecular polarity shown on the right. Another way to indicate polarity is to use the symbol δ, which means "partially." Thus, you can place δ+ over the positive atoms and δ- over the negative atoms. However, directional arrows are necessary to determine the overall molecular polarity.

Isomers: Isomers are molecules having the same formula but different molecular shapes. Usually, the presence of a C=C in a molecule can allow for "cis" and "trans" isomers if a collection of different atoms is attached to the inflexible C=C. C-C single bonds can be rotated 360^o so no cis-trans isomers are possible, but outer atoms may still be connected to different central atoms, and thus "structural isomers" are obtained. Don't confuse this phenomenon with resonance, where atoms are in the same place but a double bond can be placed in different equivalent positions between the atoms.

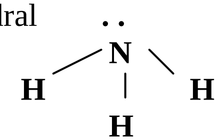
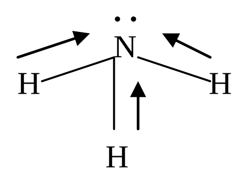
Name______________________________

Section ______________

EXPERIMENT 15: REPORT
MOLECULAR MODELS
Procedure

In the table below are a series of molecules or ions. You are to make a model of each using the model kit. Your instructor will show you how the model kit is to be used. Once the model is made, you will analyze its structure and fill in the table with the following information:

1. Indicate number of valence electrons and draw the Lewis structure. If there are resonance structures, include only one.
2. Draw the VSEPR structure and name the geometry of the electron regions
3. Name the molecular geometry and approximate bond angles.
4. Draw the VSEPR structure again, indicating the polarity of the bonds with arrows by considering the relative electronegativities of the atoms.
5. Is the molecule or ion polar overall, yes or no?
6. ***An example showing NH_3 is shown in the first set of boxes. Refer to the introduction for more info on NH_3***

Molecule or ion	**Number of Valence electrons; Lewis structure**	**VSEPR structure (AB_xE_y); geometry of electrons**	**Molecular Geometry; bond angles**	**VSEPR structure with bond polarities**	**Polar overall, yes or no?**
NH_3 example	8 H | **:**N-H | H	AB_3E_1 - total of 4 regions = tetrahedral 	trigonal pyramid < 109^o		Yes ↑
H_2O					
CH_2O (formal-dehyde)					

$SiCl_4$					
CH_2Cl_2					
H_3O^+					
NO_2^-					

IO_2^-					
SCN^- (C is the central atom)					
PO_3^{3-}					
SO_3^{2-}					

CS_2					
O_3 (ozone)					
N_3^- (azide ion)					

Discovery Question: draw all possible Lewis formulas of $C_2H_2Cl_2$ (the two C atoms are central). You may find "isomers". How are these structures different? Examine models. Predict whether each of the structures will have a molecular polarity.