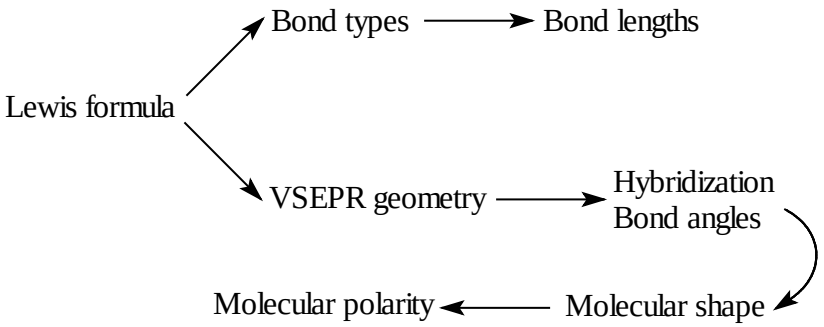
Chemistry 101 **11-MOLECULAR GEOMETRY**

In this experiment, you will build models of molecules using a model kit. These models will then be used as a guide to draw a three-dimensional representation of the molecule. This should aid you in better visualization of molecules and their bonds and structures.

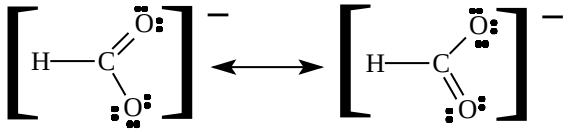
In order to establish the geometrical shapes and related aspects of molecules and molecular ions, one should first draw out the correct **Lewis formula.** From that one can determine the types and lengths of bonds, the VSEPR geometry, hybridization, bond angles, as well as the molecular shape and polarity. This is summarized in the flow chart below:



THE LEWIS FORMULA

Try to obey the octet rule when writing Lewis formulas. Some compounds, however, violate the octet rule if the central atom is a metal (such as Be or Al) or is large (such as Se, I etc.) and if the outer atoms are F or Cl. Lewis formulas do not show shape but may be used to establish the VSEPR geometry and the type of bonding (sigma, pi, or resonance).

Consider as an example the formate ion, HCO_2^-. The correct Lewis formula for the ion is shown below with its resonance structures:



The bond lengths may be calculated by adding the covalent radii of the bonded atoms. If there is a double bond or a resonance system as above, subtract 14% from the sum to obtain the correct bond length. Subtract 25% for a triple bond. For the example, the covalent radii are as follows:

C: 0.77Å H: 0.37Å O: 0.66Å

Therefore, the following bond lengths can be calculated:

H-C: 0.37Å + 0.77Å = 1.14Å

C-O resonance system: 0.77Å + 0.66Å = 1.43Å but 14% of 1.43 = 0.20Å so C-O bond length = 1.43 – 0.20 = 1.23Å

These calculations should be considered as only approximations, however.

VSEPR GEOMETRY

Using the table in your textbook as a guide, determine the VSEPR geometry for the central atom. The central atom will be designated "A", all atoms bonded to it, "B", and any non-bonded electron pairs attached to it, "E". Thus, any molecule can be represented as:

AB_xE_y (x = number of bonded atoms, y = number of nonbonded pairs of electrons)

Single, double, triple, and resonance bonds will all count the same. If there is more than one central atom, the procedure can be carried out for each one of them.

In formate ion, above, the central carbon atom is bonded to one hydrogen atom and two oxygen atoms, with no non-bonded electron pairs. It is designated $\mathbf{AB_3E_0}$. The VSEPR geometry is now assigned according to the sum (n) of x+y. In this case, the total is 3. Therefore, the VSEPR geometry is **trigonal planar**.

BUILDING THE MODELS

Select from the model kit the appropriate central piece corresponding to the total number of bonds and non-bonded pairs attached to the central atom. Insert a rigid piece for each bond or lone pair. If a double or triple bond is to be made, select flexible pieces to represent the bonds. Note that the VSEPR geometry is based on the "n" value, which counts multiple bonds the same as single bonds. The model kit is designed in such a way that models are based on total bonds and non-bonded pairs, not the value of "n". The instructor will demonstrate the kit by making a model of the formate ion.

HYBRIDIZATION AND BOND ANGLES

The VSEPR geometry leads to the bond angles and hybridization in the following way:

Value of "n"	VSEPR geometry	Bond angles	Hybridization
2	linear	180^o	sp
3	trigonal planar	120^o	sp^2
4	tetrahedral	109.5^o	sp^3
5	trigonal bipyramidal	90^o, 120^o	sp^3d
6	octahedral	90^o	sp^3d^2

DETERMINATION OF THE MOLECULAR SHAPE

If the central atom "A" has only bonds and no non-bonded pairs, the molecular shape is the same as the VSEPR geometry. However, if the central atom contains one or more lone pairs, the molecular shape will differ from the VSEPR geometry since the molecular shape represents the geometry of the atoms while the VSEPR geometry represents the geometry of all of the electron pairs attached to the central atom. This results in molecular shapes such as "bent", "see-saw", "square pyramidal", etc. You are expected to be using the text as a guide to the descriptions of molecular shapes. If the molecule has more than one central atom, a simple description of the

molecular shape can be difficult. In such a case, describe the geometry around **each central atom separately**.

MOLECULAR POLARITY

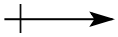
There are three factors that determine molecular polarity:

1. If the bonded atoms have different electronegativities, then the bond is polar.

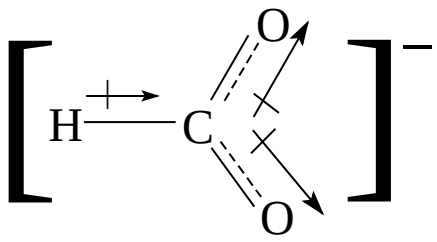
2. If the bond polarities do not cancel each other because of molecular symmetry, then the molecule is polar.

3. Bond lengths affect polarity since longer bonds can be more polar. For example, C-O is longer than C=O and is more polar. You will not be expected to consider this factor.

When a vector arrow is used to represent the polarity of a bond:

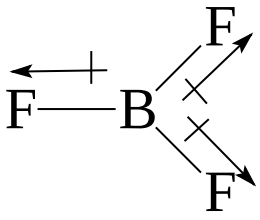


where the arrowhead is the negative end of the bond and the cross is the positive end, the formate ion can be represented as follows. The length of the arrow more or less corresponds to the electronegativity difference of the atoms.



Polarities do not cancel. The molecule is polar.

Then consider a molecule with a similar structure, BF_3:



Polarities cancel. The molecule is non-polar.

PROCEDURE

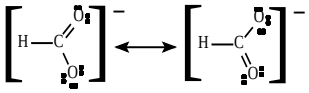
You will make models of the following molecules and draw a three-dimensional representation of their VSEPR molecular shapes into the table. If there are resonance structures, include their Lewis formulas. In some cases, you may be able to arrange the set of atoms of the formula in several different ways to form isomers. Show the structural formulas of all isomers whenever this occurs. The instructor will verify that your models and drawings are correct while you are doing the experiment.

Chemistry 101 **11-MOLECULAR GEOMETRY**

Section_____ Name_____

Report Sheet

Complete the table following the pattern given in the example.

3-D molecular drawing, with Lewis resonance structures, if necessary	**VSEPR geometry, AB_xE_y hybridization**	**Molecular shape, bond angles**	**Polarity, bond lengths**
HCO_2^- 	Trigonal planar AB_3E_0 Carbon is sp^2 hybridized	Trigonal planar HCO=120° OCO=120°	Polar C-O = 1.23Å H-C = 1.14Å
CF_4			
CHI_3			
HCl			

3-D molecular drawing, with Lewis resonance structures, if necessary	**VSEPR geometry, AB_xE_y hybridization**	**Molecular shape, bond angles**	**Polarity, bond lengths**
H_2O			
H_3O^+			
NH_3			
CS_2			
NO_2^+			

CO			

3-D molecular drawing, with Lewis resonance structures, if necessary	**VSEPR geometry, AB_xE_y hybridization**	**Molecular shape, bond angles**	**Polarity, bond lengths**
NO_2^-			
PO_4^{3-}			
C_2H_2			
P_4			

CH_3OH			
$C_2H_2Cl_2$ (all isomers)			

3-D molecular drawing, with Lewis resonance structures, if necessary	**VSEPR geometry, AB_xE_y hybridization**	**Molecular shape, bond angles**	**Polarity, bond lengths**
CH_2O			
$BeCl_2$			
BF_3			
ICl_4^-			
$SeCl_6$			

XeF_4			

Chemistry 101 **11-MOLECULAR GEOMETRY**

Section_____ Name_____

Pre-Laboratory Assignment

Fill in the table below for the indicated molecule, following the procedure given in the introduction.

3-D molecular drawing, with Lewis resonance structures, if necessary	**VSEPR geometry, AB_xE_y hybridization**	**Molecular shape, bond angles**	**Polarity, bond lengths**
PF_4^-			