Review of VSEPR and Polarity

(Chapters 9 and10 in Hill and Petrucci)
(Chapter 5 in McMurry and Castellion)
(Chapters 8 and 9 in Brown and LeMay)
(Chapter 9 in Kotz)

• In order to discuss topics in organic chemistry, we must remember some information about molecular geometry and polarity. In essence, we need to review Valence Shell Electron Pair Repulsion Theory (VSEPR) (Chapter 10, Sections 10.1 and 10.2 (Hill)).

• In order to understand VSEPR you must remember how to write Lewis Structures (Chapter 9 (Hill), Chapter 5, (Sections 5.5-5.9 McMurray), or Chapters 8 and 9 (Brown and LeMay). If you are rusty on Lewis Theory, please review the sections listed and do the Examples and Exercises within these sections.

I. VSEPR

• Lewis Theory allows us to predict how atoms are bonded to each other. VSEPR allows for the prediction of the "3-D shape of a molecule," or, what is better known as the molecular geometry.

> Molecular geometry: The geometric shape of a molecule (the arrangement of a molecule's atoms in 3-D space).

• To discuss the molecular geometry of the molecule we must also discuss the electron group geometry.

> Electron group geometry: the arrangement of electron pairs-both bonding and nonbonding (lone pairs)-about a central atom.

• VSEPR assumes two general rules: 1) electron pairs (both bonding and nonbonding) around the central atom attempt to be as far as apart as possible and 2) double and triple bonds can be treated as though they were a single bond.

• Once the electron group geometry has been determined the molecular geometry can be determined. If no lone pairs are present, the electron group geometry and the molecular geometry will be the same.

• Here are some general guidelines for determining the electron pair geometry and molecular geometry of a molecule.

1) Write the Lewis structure of the molecule or polyatomic ion.

2) Determine the number of bonding pairs and lone pairs around the central atom, then assume that these pairs of electrons will want to be as far apart as possible.

3) Identify the spatial orientation of the electron pairs around the central atom i.e. linear, tetrahedral, etc. (See the additional handout for possible special orientations). You now have determined the electron group geometry.

4) To determine the molecular geometry, determine the geometrical shape of the molecule based on the position of the outlying atoms around the central atom. (Again see the additional handout for the names of these molecular geometries).

II. Polarity

• The molecular geometry of the molecule now dictates the polarity of the molecule.

• A molecule is considered polar if it has an overall molecular dipole.

Molecular dipole: a charge separation in a molecule (permanent partial charges, δ^- and δ^+).

• In order to predict whether a molecule has a molecular dipole you must determine whether the molecule contains polar bonds.

• Polar bonds occur when the electrons in a chemical bond are attracted to the more electronegative atom.

Electronegativity: The ability of an atom to attract bonding electrons to itself.

• Polar bonds create bond dipoles. If these bond dipoles do not cancel out, then the molecule has a molecular dipole. This is where molecular geometry plays a role in determining the polarity of a molecule.

Ex: HCl
H_2O
CO_2
CCl_4
N_2