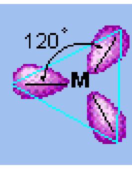
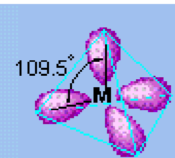
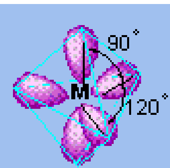
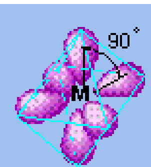
Molecular Structure

Molecular Structure: The three-dimensional arrangement of the atoms comprising a molecule

- Bond Angle: The angle between any two bonds that include a common atom.
- Bond Distance: The distance between the nuclei of two bonded atoms.

Valence Shell Electron Pair Repulsion Theory: Method for predicting molecular structures

Number of Regions	Spatial Arrangement	Electron-Pair Geometry
Two regions of high electron density (bonds and/or unshared pairs)		**Linear.** 180° angle.
Three regions of high electron density (bonds and/or unshared pairs)		**Trigonal planar.** All angles 120°.
Four regions of high electron density (bonds and/or unshared pairs)		**Tetrahedral.** All angles 109.5°.
Five regions of high electron density (bonds and/or unshared pairs)		**Trigonal bipyramidal.** Angles of 90° or 120°. An attached atom may be equatorial (in the plane of the triangle) or axial (above or below the plane of the triangle).
Six regions of high electron density (bonds and/or unshared pairs)		**Octahedral.** All angles 90° or 180°.

Bonding & Nonbonding Electron Pairs

- The presence of unshared electron pairs affect molecular structure.
- Electron pair geometry: Geometry which includes all electron pairs.
- Molecular geometry: The structure that includes only the placement of atoms in the molecule.
- Structures are the same if there are no unshared pairs.
- Structures differ with unshared pairs.
- Both shared (bonding) and unshared (nonbonding) electron-pairs form regions of high electron density.
- Electrostatic repulsion pushes these electron dense regions as far apart as possible.
- Small distortions may occur due to differences in electrostatic strengths.

Rules for Predicting Electron-Pair and Molecular Geometry

- Draw the Lewis Structure
- Determine the number of regions of high electron density
- Determine the most stable arrangement
- Identify the molecular structure

Molecular Polarity

- Polar molecules: Any molecule having one positive and one negative end.
- Polar molecules occur due to the formation of polar bonds.
    - Positive end: σ+
    - Negative end: σ–
- Dipole moment: A measure of the polarity of a molecule.

Valence Bond Theory -- Hybridization of Atomic Orbitals

Hybridization: The mixing of atomic orbitals of an isolated atom to form hybrid orbitals

Orbital overlap: A portion of two orbitals overlapping the same region of space

Sigma Bonds (σ bonds): A covalent bond in which the electron density is concentrated in the region between the two nuclei.

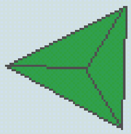
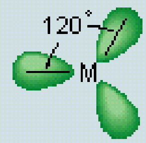
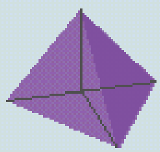
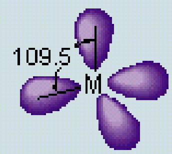
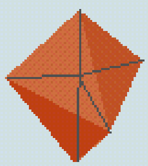
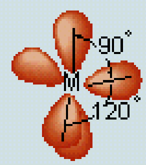
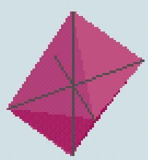
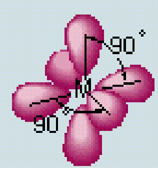
Pi Bonds (π bonds): A covalent bond in which the electron dense regions overlap above and below the internuclear axis.

Types of Hybridization: Sp, Sp^2, Sp^3, Sp^3d, $Sp^3d^{\,2}$, or Sp^3d^2

Assigning Hybrid Orbitals

- Determine the Lewis structure
- Determine the electron-pair geometry
- Assign a set of hybridized orbitals

Remember!!! --- Only sigma bonds form hybrid orbitals

Regions of Electron Density		Arrangement	Hybridization	
2		Linear	sp	
3		Trigonal planar	sp^2	
4		Tetrahedral	sp^3	
5		Trigonal bipyramidal	sp^3d	
6		Octahedral	sp^3d^2	

Hybridization also involving double & triple bonds

Double bonds have one sigma and one pi bond, while triple bonds have one sigma and two pi bonds.