Chemistry 1000 Lecture 16: Molecular shape

Marc R. Roussel

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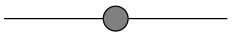
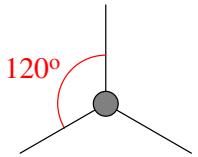
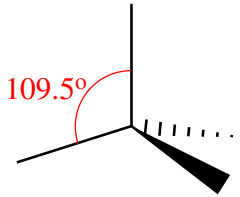
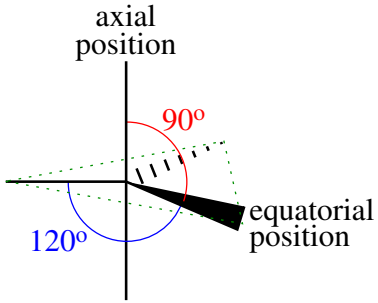
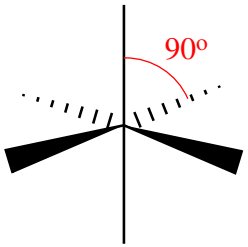
Valence Shell Electron Pair Repulsion Theory

- Developed in the mid-20th century by Sidgwick, Powell, Nyholm and Gillespie (McMaster University professor and U. of L. honorary degree recipient)
- Key ideas:
  - Electrons repel.
  - Valence electrons (bonding and nonbonding) are particularly close together at an end of a bond near a central atom.
  - Electrons can be thought of as "living in groups" of nonbonding electron lone pairs and covalent bonds.
    - A bond of any order (single, double triple) is a single group.
  - The electronic geometry around an atom is therefore dictated by the mutual repulsion of electron groups near that atom.
  - Electrons organize themselves so as to minimize the repulsion between groups.

Basic VSEPR Geometries

Number of groups	Shape	Name
2		linear
3		trigonal planar
4		tetrahedral
5		trigonal bipyramidal
6		octahedral

Examples

CO_2, CH_4, PCl_5, SF_6

Lone pairs

- Lone pairs are "fatter" than bonding pairs.

Consequences:

1. Lone pairs locate themselves where there is the most space.
2. Lone pairs push the bonding electrons away, distorting their geometry away from the ideal geometry for n identical electron groups.

- To name geometries of molecules with lone pairs, first determine the electronic geometry as one of the basic VSEPR geometries.

- Then look at the shape made by the atoms surrounding the central atom and name this shape.

- The names of the shapes derived from the basic VSEPR geometries will be given in the following examples:
  NH_3, H_2O, SF_4, ClF_3, ClF_5, XeF_4
  (Discuss bond angles in each case.)

Larger molecules

- We can apply VSEPR theory to each non-terminal atom.
- Sometimes, geometric constraints mean that we can't obtain the "ideal" VSEPR geometry.

Examples: C_2H_4, CH_3CN, cyclopropane (C_3H_6)

Bond polarity

- A dipole is a pair of equal and opposite charges separated by a distance d.
- The strength of a dipole is measured by the dipole moment,

$$\mu = qd$$

- Polar bonds can be thought of as little dipole vectors.
  By convention in chemistry, these vectors point toward the negative (more electronegative) end of a bond.
  This is contrary to the convention in physics.

Molecular polarity

- The overall dipole moment of a molecule is the vector sum of the bond dipoles.
- A molecule with a nonzero dipole moment is said to be polar.
  A molecule with a zero dipole moment is nonpolar.
- The positive and negative ends of a molecule are often labeled with the symbols $\delta+$, $\delta-$ rather than drawing dipole moment vectors.

Examples: HCl, CO_2, O_3, BF_3, CH_4, CH_3Cl, NH_3, SF_4, PCl_5, C_2H_6, CH_3CHO