Accelerated General Chemistry
Chapter 3: Molecular Geometry (in Atkins and Jones)

- Goal: Convert a Lewis structure of a species into its three-dimensional structure:
  - <u>Shape</u> (an overall description)
  - <u>Bond Angles</u>
  - [Trends in bond lengths]

- Realize goal with **<u>Valence Shell Electron Pair Repulsion (VSEPR) Theory</u>**
  - Electron groups around an atom repel each other
  - Therefore, maximize the angles between electron groups

- Two key terms (not explicitly defined in Atkins and Jones):
  - <u>Coordination Number</u> (CN) = the number of atoms (also known as substituents) bonded to a given atom
  - <u>Steric Number</u> (SN) = the number of electron groups around a given atom
    SN = CN + (the number of lone pairs) + (the number of unpaired electrons)
  - CN and SN can be determined for any atom in a species (not just a central atom)

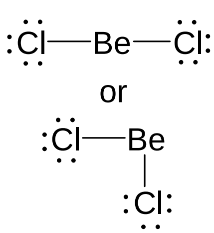
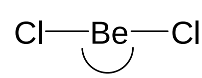
- Need both SN and CN to fully define a molecule's shape

VSEPR Theory for Compounds with Normal Valences

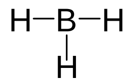
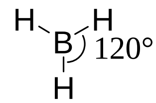
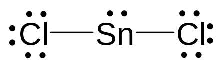
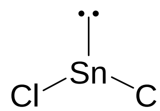
(most relevant to Organic Chemistry next year)

You must memorize all of the following ideal bond angles,
electron group arrangements, and shape names

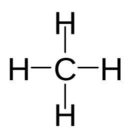
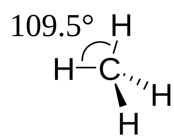
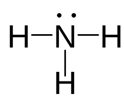
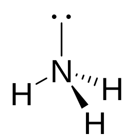
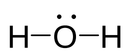
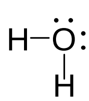
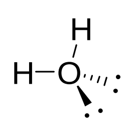
SN = 2 Ideal Bond Angle = 180º
Electron Group Arrangement: linear

Possible CN's	Lewis Structure *e.g.*	Shape	Shape Name
CN = 2		 180°	linear

SN = 3 Ideal Bond Angle = 120º
Electron Group Arrangement: trigonal planar

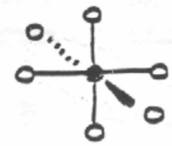
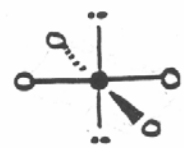
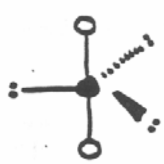
Possible CN's	Lewis Structure *e.g.*	Shape	Shape Name
CN = 3			trigonal planar
CN = 2	 (large Group 14 can have less than an octet)		bent (or angular) (names based on atom locations only)

SN = 4 Ideal Bond Angle = 109.5º
Electron Group Arrangement: tetrahedral

Possible CN's	Lewis Structure *e.g.*	Shape	Shape Name
CN = 4			tetrahedral
CN = 3			trigonal pyramidal
CN = 2	 or 		bent (or angular) (but how similar is it to $SnCl_2$?)

If for a given atom (1) SN = CN and (2) all substituents are identical, the actual (experimental) bond angles will be the same as the ideal bond angles (by symmetry).

VSEPR Theory for Hypervalent Compounds

S.N.	C.N.	Shape Names (ideal bond angles)	S.N.	C.N.	Shape Names (ideal bond angles)
5	5	 Trigonal bipyramidal 90°, 120°	6	6	 Octahedral 90°
	4	 See-saw 90°, 120°		5	 Square pyramidal 90°
	3	 T-shaped 90°		4	 Square planar 90°
	2	 Linear 180°			

Ideal Bond Angle = 90º

Electron Group Arrangement: octahedral

Ideal Bond Angles = 90º, 120º (180° for linear)

Electron Group Arrangement: trigonal bipyramidal

You are not required to memorize the shape names for SN = 5 and SN = 6. However, you should be able to explain the shapes and bond angles.