

## Chapter 10: Molecular Geometry

- Goal: Convert a Lewis structure of a species into its three-dimensional structure:
  - Shape (an overall description)
  - Bond Angles
  - [Trends in bond lengths]
- Realize goal with **Valence Shell Electron Pair Repulsion (VSEPR) Theory**
  - Electron groups around an atom repel each other
  - Therefore, maximize the angles between electron groups
- Two key terms (not explicitly defined in Silberberg):
  - Coordination Number (CN) = the number of atoms (also known as substituents) bonded to a given atom
  - Steric Number (SN) = the number of electron groups around a given atom  
 $SN = CN + (\text{the number of lone pairs}) + (\text{the number of unpaired electrons})$
  - 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 =  $180^\circ$   
 Electron Group Arrangement: linear

Possible CN's	Lewis Structure <i>e.g.</i>	Shape	Shape Name
<b>CN = 2</b>	$\begin{array}{c} \text{:}\ddot{\text{Cl}}\text{---Be---}\ddot{\text{Cl}}\text{:} \\ \text{or} \\ \text{:}\ddot{\text{Cl}}\text{---Be} \\   \\ \text{:}\ddot{\text{Cl}}\text{:} \end{array}$	$\begin{array}{c} \text{:}\ddot{\text{Cl}}\text{---Be---}\ddot{\text{Cl}}\text{:} \\ \text{180}^\circ \end{array}$	linear

**SN = 3**    Ideal Bond Angle =  $120^\circ$   
 Electron Group Arrangement: trigonal planar








Possible CN's	Lewis Structure <i>e.g.</i>	Shape	Shape Name
<b>CN = 3</b>	$\begin{array}{c} \text{H}-\text{B}-\text{H} \\   \\ \text{H} \end{array}$		trigonal planar
<b>CN = 2</b>	$\begin{array}{c} :\ddot{\text{Cl}}-\ddot{\text{Sn}}-\ddot{\text{Cl}}: \\ \text{(large Group 4A can have} \\ \text{less than an octet)} \end{array}$		bent  (names based on atom locations only)

**SN = 4**    Ideal Bond Angle =  $109.5^\circ$   
 Electron Group Arrangement: tetrahedral

Possible CN's	Lewis Structure <i>e.g.</i>	Shape	Shape Name
<b>CN = 4</b>	$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{H} \\   \\ \text{H} \end{array}$		tetrahedral
<b>CN = 3</b>	$\begin{array}{c} \text{H}-\ddot{\text{N}}-\text{H} \\   \\ \text{H} \end{array}$		trigonal pyramidal
<b>CN = 2</b>	$\begin{array}{c} \text{H}-\ddot{\text{O}}-\text{H} \\ \text{or} \\ \text{H}-\ddot{\text{O}}: \\   \\ \text{H} \end{array}$		bent  (but how similar is it to SnCl <sub>2</sub> ?)

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

<u>S.N.</u>	<u>C.N.</u>	Shape Names (ideal bond angles)	<u>S.N.</u>	<u>C.N.</u>	Shape Names (ideal bond angles)
5	5	 Trigonal bipyramidal $90^\circ, 120^\circ$	6	6	 Octahedral $90^\circ$
	4	 See-saw $90^\circ, 120^\circ$		5	 Square pyramidal $90^\circ$
	3	 T-shaped $90^\circ$		4	 Square planar $90^\circ$
	2	 Linear $180^\circ$			

Ideal Bond Angle =  $90^\circ$   
 Electron Group Arrangement:  
 octahedral

Ideal Bond Angles =  $90^\circ, 120^\circ$   
 ( $180^\circ$  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.