Chapter 10: Chemical Bonding II: Molecular Geometry and Bonding Theory

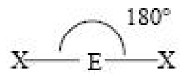
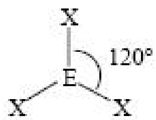
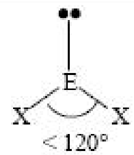
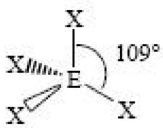
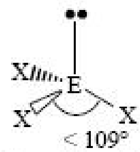
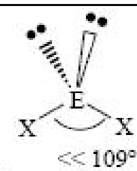
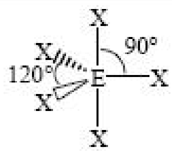
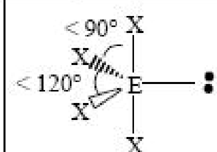
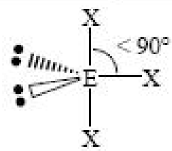
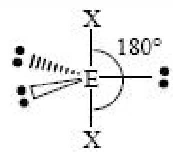
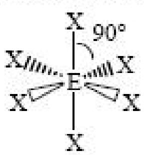
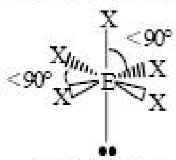
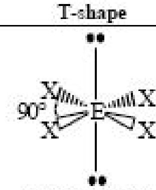
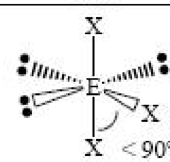
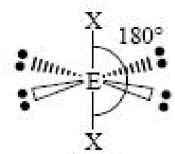
Ionic bonding: crystal lattice
Covalent bonding: VSEPR, valence bond and hybridization theory
Metallic bonding: ability of electrons to flow on all atoms.

VSEPR: Valence shell electron pair repulsion theory.

Electrons try to be as far away from each other as possible. In bonding and bonding theory only the valence electrons are important. Each geometry is associated with its bond angles.
Molecular geometry can be as follows:
(A = central atom, X = terminal atoms and E = lone pair of electrons)

Electron Groups	AXE formula	Bond Angle	Example	Electronic Geometry	Shape of Molecule
2	AX_2	180^o	$BeCl_2$	Linear	Linear
3	AX_3	120^o	BF_3	Trigonal planar	Trigonal planar
3	AX_2E	120^o	SO_2	Trigonal planar	Bent
4	AX_4	109.5^o	CH_4	Tetrahedral	Tetrahedral
4	AX_3E	109.5^o	NH_3	Tetrahedral	Trigonal Pyramidal
4	AX_2E_2	109.5^o	H_2O	Tetrahedral	Bent
5	AX_5	90^o, 120^o, 180^o	PCl_5	Trigonal bipyramidal	Trigonal Bipyramidal
5	AX_4E	90^o, 120^o, 180^o	SF_4	Trigonal bipyramidal	Seesaw
5	AX_3E_2	90^o, 180^o	CIF_4	Trigonal bipyramidal	T – shape
5	AX_2E_3	180^o	XeF_2	Trigonal bipyramidal	Linear
6	AX_6	90^o, 180^o	SF_6	Octahedral	Octahedral
6	AX_5E	90^o	BrF_5	Octahedral	Square Pyramidal
6	AX_4E_2	90^o	XeF_4	Octahedral	Square Planar
6	AX_3E_3	90^o, 180^o		Octahedral	T – Shape
6	AX_2E_4	180^o		Octahedral	Linear

Figure on the next page.

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal Planar	 Bent or Angular			
4	 Tetrahedral	 Trigonal Pyramid	 Bent or Angular		
5	 Trigonal Bipyramid	 Sawhorse or Seesaw	 T-shape	 Linear	
6	 Octahedral	 Square Pyramid	 Square Planar	 T-shape	 Linear

(*from: http://justonly.net/blog/2011/03/chem-201-shapes-of-molecules/)*

Dipole moment and polar molecules

- Polar bond and polar molecules
- Polar bond – when the two atoms of a bond have different electronegativity while
- Polar molecules have overall non-zero dipole moments and non polar molecules have zero dipole moment.
- A bond can be polar but the molecule does not have to be.
- Dipole moment = magnitude of charge x distance separating the positive and negative charge
- Units (debye = coulomb x meter)
- Dipole moment usually can be determined by exposing molecules to electric field.

Determining the polarity of a molecule

1) write Lewis structure of molecule (write ALL electrons)
2) write the shape of molecule
3) check the electronegativity of each atom (estimate from PT)
4) see the symmetry of the molecule (not just in shape but in types of atoms)
5) see if the equal electronegativity of similar atoms cancel each other out, if not then molecule may be polar.

Valence Bond Theory
Electron clouds of opposite spins overlap to form bonds. Important points:

a) Electrons stay in their respective orbitals
b) Bonding electrons localize in the region of overlap
c) Maximum overlap occurs when orbitals overlap end to end
d) Molecular geometry depends on geometry of orbitals.

Has flaws when looking at bond angles and molecular of majority of molecules.

Hybridization
Mixing of orbitals of excited atoms to form new orbitals, which overlap to form bonds.

Type	Typical shape	Bond angle	e.g.
Sp^3	Tetrahedral	109^o	CH_4, HN_3
Sp^2	Trigonal planar	120^o	BF_3, $CH_2{=}CH_2$
Sp	Linear	180^o	BeF_2, $CH\equiv CH$

Hybrid orbitals of d shell are also possible.

Hybridization in organic chemistry
Alkanes, alkenes, alkynes.
Geometric isomerism: cis and trans geometry of alkenes.

Molecular Orbital Theory
Atomic orbitals (AO) combine to form molecular orbitals (MO) and antibonding molecular orbitals.