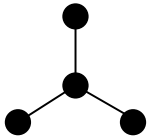
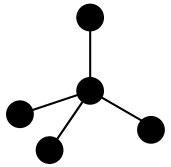
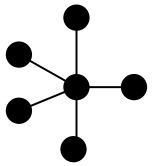
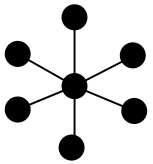
Chemistry 102 – Basic Geometries, Bond Angles, Shapes and Hybridization

# electron groups	Bond angle	Base geometry	# lone pairs	Shape		Hybridization
2	180°	Linear	0	Linear		sp
3	120°	Trigonal planar	0	Trigonal planar		sp^2
			1	Bent		
4	109.5°	Tetrahedral	0	Tetrahedral		sp^3
			1	Trigonal pyramidal		
			2	bent		
5	90°/120°	Trigonal bipyramidal	0	Trigonal bipyramidal		sp^3d
			1	See-saw		
			2	t-shaped		
			3	Linear		
6	90°	Octahedral	0	Octahedral		sp^3d^2
			1	Square pyramidal		
			2	Square planar		

To assign bond angle, shape and hybridization:

1. Draw the Lewis dot structure.
2. Consider the central atom (or the atom of focus for more complex molecules) and determine:
    a. How many bonded atoms
    b. How many lone pair(s) on this atom
3. Based on this, determine the number of electron groups.
4. Using the number of electron groups, determine the **bond angle**.
5. Consider again the number of lone pairs on the central atom – these are not considered in the shape. Use the base geometry and include the number of lone pairs to determine the **shape** of the molecule.
6. Using the number of electron groups, how many hybrid orbitals are needed (remember, each bond contains a σ component). All sigma bonds and lone pairs of electrons use hybrid atomic orbitals. This gives you the **hybridization**.

1. To determine the *polarity*, again consider the Lewis dot structure and bond angle (so do numbers 1-4).
2. Assign polarity to the bonds – bonds are either nonpolar (homonuclear – same element) or polar (heteronuclear – different elements). The direction of the bond moment is assigned using electronegativity (towards the more electronegative element) and this is based on periodic trends.
3. Assign polarity to the molecule:
    a. Even distribution of electron density (all polar bonds cancel – can think about this like vector addition) – *nonpolar molecule*
    b. Uneven distribution of electron density (all polar bonds do not cancel) – *polar molecule*
4. Show the direction of the dipole moment for polar molecules.

Molecular Orbital Configurations:

1. Give/Fill in the electron configuration for each atom in the molecule. Remember to add or subtract for ionic charges.
2. Fill in the molecular orbital configuration based on:
    a. Pauli's exclusion principle (only two electrons per molecular orbital)
    b. Aufbau principle (fill in the lowest to highest energy)
    c. Hund's rule (fill in degenerate orbitals to yield the greatest number of unpaired same spins)
3. Determine bond order based on:
    a. Bonding electrons (lower in energy than their atomic orbitals, noted without a "*")
    b. Antibonding electrons (higher in energy than their atomic orbitals, noted with a "*")
    c. Subtract and divide by two. Bond order correlates to the number of bonds we draw with Lewis dot structures. Bond orders can be fractions.