The Octet Rule!!!!!!

Chemical compounds form in a way so that each atom can have an octet (8) of electrons in the highest energy level. This is accomplished by **gaining, losing, *or* sharing** *electrons.*

Hydrogen, Beryllium and Boron are exceptions to the octet rule. Be and B will be discussed later. For now let's look at hydrogen.
H only has one electron and energy level one can only hold 2 electrons max.
So H forms bonds in which it is surrounded by only two electrons.

Let's look at the bonding, Lewis structure and structural formulas for some simple molecules.

Molecular Formula	Bonding	Lewis Structure	Structural Formula
H_2			
HCl			

Molecular Formula	Bonding	Lewis Structure	Structural Formula
O_2			
N_2			

When drawing Lewis Structures, it is good to know the following guidelines:

1. Molecules are usually as symmetrical as possible. This gives an even distribution of charge.
2. If carbon is present, it will usually be the center of the molecule.
3. Carbon, nitrogen, oxygen and fluorine never break the octet rule.

Here is a handy method for drawing Lewis structures. It is called "Needs, Available, Shared".

1. Calculate the total number of electrons "needed" by the atoms in the molecule. Remember, every atom "needs" an octet except hydrogen, beryllium and boron. Hydrogen is stable with two electrons.

Needs = [# of atoms (other than hydrogen) in the molecule x 8] + [# of hydrogen atoms in the molecule x 2]

2. Calculate the total number of electrons "available" to the molecule. This is the total of all the valence electrons in all the atoms

Available = total # of valence electrons in all atoms

3. Calculate the number of electrons shared between atoms.

Shared = Needs minus Available

4. Calculate the number of electrons not shared.

Not Shared = Available minus Shared

Use "Needs, Available, Shared" to help you draw correct Lewis structures for the following molecules:

a.) **IBr**

b.) **CH_3Br**

c.) **C_2HCl**

d.) **F_2O**

Polyatomic Ions – a group of covalently bonded atoms that has a charge. An electron has been gained by the group or lost from the group. Polyatomic ions form ionic bonds with oppositely charged ions.

You can use Needs, Available, Shared to help you draw Lewis structures for polyatomic ions too. Just add or subtract the appropriate number of electrons to the Available number. Brackets are placed around the Lewis structure and the charge is placed outside the brackets.

NH_4^+ (ammonium ion)

NO_3^- (nitrate ion)

Resonance – a phenomenon that exists when more than one Lewis structure can be drawn for a species. These structures are known as contributing resonance structures and are usually illustrated together and separated by a double arrow. The actual structure of the species is a blend (average) of its contributing resonance structures. The arrows do not mean that the molecule "flips" from one structure to another.

SO_3

NO_2

Odd-Electron Molecules

Molecules that have Lewis Structures with an unpaired electron are often called free radicals. The unpaired electron makes the molecule unusually reactive. Free radicals have been implicated in such biological processes as aging and cancer. In an effort to pair up the single electron, free radicals may also form dimmers or pairs of molecules. For example, the molecule NO_2 dimerizes to produce the N_2O_4 molecule in the reaction

$$2NO_2 \rightarrow N_2O_4$$

Lewis structure of the NO_2 molecule:

The localized electron model is based on pairs of electrons, it does not handle odd electron molecules in a natural way. To treat odd electron molecules, a more sophisticated model is needed.

Formal Charge – an arbitrary scheme for assigning charges to the atoms in a polyatomic ion or molecule. These charges are not real, but they do serve purpose in weeding out unfavorable structures. Formal charge is determined by finding the difference between the number of electrons on the free atom and the number of valence electrons assigned to the atom in a molecule.

The rules for assigning a formal charge to an atom are as follows:

1. All lone pairs of electrons, L, are assigned solely to that atom.
2. The atom is also assigned one-half the number of shared pairs of electrons, S.
3. If V is the number of valence electrons in the unbonded atom, then the atom's formal charge, FC, is

The assignment of one-half of the shared electrons to each atom in a bonded pair indicates that formal charge stresses the covalent nature of each of the bonds.

Remember the following guidelines:

1. The formal charges should be as close to 0 as possible.
2. The negative formal charges should reside on the most electronegative atoms.
3. Adjacent atoms should not have formal charged with like signs
4. The sum of the formal charges of all atoms in a given molecule or ion must equal the overall charge of that species.

Examples:

Final note (some cautions about formal charges): Although formal charges are closer to actual atomic charges in molecules than are oxidation states, formal charges still provide only <u>estimates</u> of charge - they should not be taken as actual atomic charges. Also, the evaluation of Lewis structures using formal charges can lead to erroneous predictions.

Sigma and Pi Bonds

All single bonds are sigma (   ) bonds. They are formed by the "head to head" overlap of two merging atomic orbitals. The merged orbitals have a symmetry about the bond axis.

Sigma bonds form when an s orbital overlaps another s orbital
an s orbital overlaps a p orbital
a p orbital overlaps another p orbital

Pi (   ) bonds form from the "side by side" overlap of two p orbitals. Each pi bond is double-lobed, lying above and below the internuclear axis.

Single covalent bond = 1 sigma bond
Double covalent bond = 1 sigma bond and 1 pi bond
Triple covalent bond = 1 sigma bond and 2 pi bonds