# CHEMISTRY & MATERIALS SCIENCE

## Introduction

### Stoichiometry

All stoichiometric equations for quantities may be derived from

$$n_1/v_1 = n_2/v_2 \tag{1}$$

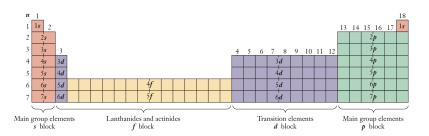
The percentage yield is defined as

% yield = 
$$\frac{\text{actual yield}}{\text{theo. yield}} \times 100\%$$
 (2)

A crucial aspect in confirming stoichiometric results is using dimensional analysis; that is, using the dimensions of each unit in the equation(s) and confirming the final unit has the proper dimensions.

### Bonding

The total number of orbitals is equal to  $n^2$ , where n is the principle quantum number, wherein each orbital has a maximum of two electrons. This maximum occurs only if all subshells contain one electron originally, known as Hund's rule.



The formal charge is given by  $q_f = n_v - n_l - \frac{1}{2}n_s$  in which  $\sum q_f = 0$ . Hybrid orbitals are dependent on molecular geometry, and filled by  $sp^3d^2$ . The number of orbitals is equal to the number of electron pairs. The number of sigma and pi bonds is equal to

$$n_{\sigma} = \sum n_{\rm all}$$
 and  $n_{\pi} = \sum n_{\rm dbl} + 2\sum n_{\rm tri}$  (3)

moles n = m/M = CVatoms  $n_{\text{atoms}} = \rho V N_a / M$ molarity C = mn/MVdilution  $n_1 = n_2$ 

Figure 1: Equations for quantities derived from Equation 1.

The orbitals are filled in the order of  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 ...$ 

 $n_v$  is the total number of valence electrons;  $n_l$  is the number of lone pairs; and  $n_s$  is the number of electrons shared in bonds.

### Atoms & Molecules

Other properties of the periodic table include

- Atomic size increases toward the bottom left;
- Ionization energy and electronegativity increase towards the top right;

Lewis dot structures are created via the following algorithm:

- 1. Count the total number of valence electrons in the molecule;
- 2. Place single bonds between all connected atoms;
- 3. Place the remaining valence electrons not accounted for in (2) on individual atoms, specifically as lone pairs whenever possible;
- 4. Create multiple bonds as needed for any atoms that do not have a full octet



Figure 2: The seesaw VSEPR model constructed from a lewis diagram.

# Chemical Equilibrium

### *Equilibrium Constants*

A system is said to be at dynamic equilibrium if the rates of both reactions are equal but do not approach zero. For a general chemical reaction, the reaction quotient and equilibrium constant are

$$Q = \frac{[C]^{c}[D]^{d}}{[A]^{a}[B]^{b}} \quad \text{and} \quad K_{c} = \frac{[C]^{c}_{eq}[D]^{d}_{eq}}{[A]^{a}_{eg}[B]^{b}_{eg}}$$
(4)

respectively. For reactions which take place in the gas phase,

$$K_p = K_c R T^{\Delta n_g} \iff [X] \equiv P_X = [X] R T$$
 (5)

where  $\Delta n_g = c + d - (a + b)$ . Reactions are homogeneous iff all constituents are either exclusively gaseous or aqueous. Incidentally, in a heterogeneous reaction, K only includes the compounds in the reaction which are not solid nor liquid. For a series of reactions,

$$K_n = \prod K_i \tag{6}$$

A general equilibrium reaction is given by aA + bB = cC + dD, where a, b, ... are the stoichiometric coefficients v.