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CHEMISTRY & MATERIALS SCIENCE

Introduction

Stoichiometry

All stoichiometric equations for quantities may be derived from

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

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

Figure 1: Equations for quantities derived from Equation 1.

The percentage yield is defined as

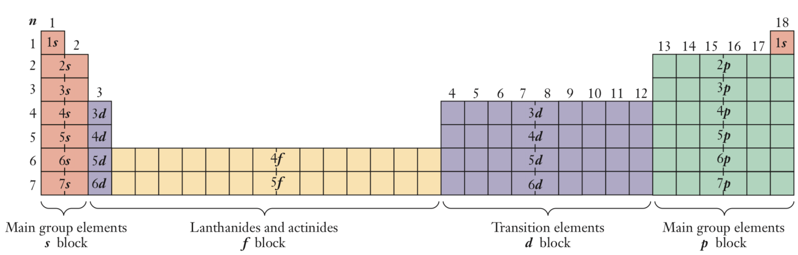
$$\%\ \text{yield} = \frac{\text{actual yield}}{\text{theo. yield}} \times 100\% \tag{2}$$

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



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_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.

$$n_\sigma = \sum n_{\text{all}} \quad \text{and} \quad n_\pi = \sum n_{\text{dbl}} + 2\sum n_{\text{tri}} \tag{3}$$

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;

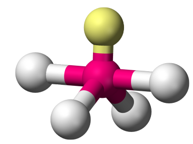


Figure 2: The seesaw VSEPR model constructed from a lewis diagram.

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

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

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

$$Q = \frac{[C]^c[D]^d}{[A]^a[B]^b} \quad \text{and} \quad K_c = \frac{[C]^c_{eq}[D]^d_{eq}}{[A]^a_{eq}[B]^b_{eq}} \tag{4}$$

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

$$K_p = K_c RT^{\Delta n_g} \iff [X] \equiv P_X = [X]RT \tag{5}$$

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,

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

R	A	A'	B
I	$[A_i]$	$[A'_i]$	$[B_i]$
C	$-ax$	$-a'x$	$+bx$
E	$[A]_{eq}$	$[A']_{eq}$	$[B]_{eq}$

Figure 3: Calculating concentrations for a reaction at equilibrium.

The procedure to calculate final concentrations of specific compounds in a reaction $A \leftrightharpoons B$ is as follows:

1. For reactants and products, $[A_i]_{eq} = [A_i] \mp ax$, respectively.

2. Using these concentrations in K, solve for x.

3. Substitute x into the original equilibrium concentrations.