Chem 7/11 Equations In Large X

Stoichiometry & Aqueous Solutions

The mole counts numbers of atoms or molecules using mass.

1 mole = A.N. = 6.02×10^{23} entitities Mol X = $\frac{grams X}{Molar Mass X}$

% Yield = $\frac{experimental\ mass}{theoretical\ mass} \times 100$

% Mass ↔ Chemical Formula

% mass of Element $X = \frac{mol \ X \ in \ formula \times molar \ mass/1 \ mol \ X}{mass \ of \ 1 \ mol \ compound}$

Molarity is a common concentration unit in aqueous chemistry. The dilution equation is used for the preparation of solutions using stock solutions.

 $\mathsf{molarity} = \mathsf{M} = \frac{\mathsf{moles \ solute}}{\mathsf{L \ solution}} \qquad \qquad M_1 V_1 = M_2 V_2$

Gases

The ideal gas law describes the behavior of gases at low pressure and high temperatures.

PV = nRT $\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2}$ (move constants to one side variables to another)

The gas law can be expressed as a function of molar mass and gas density.

 $MolarMass = \frac{mRT}{VP} = \frac{dRT}{P}$ 0.0821 L atm/mol K and T in Kelvin

Dalton's Law: P_{Total} of a mixture of gases is the sum of the partial pressures.

$$P_{total} = \mathsf{P}_1 + \mathsf{P}_2 + \mathsf{P}_3 + \dots$$

Thermochemistry

Internal and energy and enthalpy are state functions

 $\Delta \mathsf{E} = q + w = q - P \Delta V \qquad \Delta H = q_p = \Delta E + P \Delta V \qquad \Delta \mathsf{H}_{rxn}^\circ = \Delta \mathsf{H}_{products}^\circ - \Delta \mathsf{H}_{reactants}^\circ$

Standard State is a specified experimental conditions of 1 atm ideal gas, 1M liquids and 298K.

Hess' Law and ΔH_f° values allows computation of ΔH_{rxn}° standard state conditions.

 $\sum n_i \Delta H^{\circ}_{if}(products)$ - $\sum m_j \Delta H^{\circ}_{jf}(reactants)$

Quantum Theory

Energy is quantized at the molecular level. The speed of light in a vacuum is constant.

 $E = h\nu$ h = 6.63 × 10⁻³⁴ J sec $c = \lambda \nu = 3.0 \times 10^8 m/s$

IMF's and Solutions

The heat an object gains or loses is proportional to its mass and the change in temperature.

 $q = Mass \times Spefic Heat Capacity \times \Delta T$ OR $q = \# Moles \times Molar heat capacity \times \Delta T$

The heat of fusion and vaporization are heats required or given off during phases changes.

 $q = \# Moles \times \Delta H_{fusion}$ and $q = \# Moles \times \Delta H_{vaporization}$

When calculating heat changes in matter the conservation of energy is obeyed.

 $\sum q_i = q_{heating \ solid} + q_{melting \ solid} + q_{heating \ liquid} + q_{vaporizing \ liquid} + q_{heating \ gas}$

The Clausius-Clayperon relates the vapor pressure P_1 at T_1 to the vapor pressure P_2 at T_2 .

 $\ln \frac{P_2}{P_1} = \frac{-\Delta H_{vap}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \quad \text{where R is 8.314 J mol}^{-1} \text{ K}^{-1}.$

The solubility of a gas in a liquid is equal to the partial pressure of that gas above the liquid times the Henry's Law constant for that gas/solvent combination.

 $S = k_{Henry} \times P_i$

Raoult's Law: The partial pressure of a vapor over its liquid is equal to the mole fraction of the solvent times the vapor pressure of the pure liquid.

$$P_{vapor} = \chi_{solvent} \ P_{solvent}^{\circ}$$

Colligative properties are physical properties that depend only on the number of solute molecules dissolved in a solvent (and not the chemical identity of the solute).

BP Elevation	FP Depression	Vapor Pressure Lowering	Osmotic Pressure
$\Delta T_b = (T_b - T_b^\circ) = m \; K_b$	$\Delta T_f = -(T_f - T_f^\circ) = m \; K_f$	$\Delta P_{vapor} = \chi_{solute} \; P^\circ_{solvent}$	$\pi = M R T$

Concentration Units

Chemistry uses many units to specify concentration.

 $molarity = M = \frac{moles \text{ solute}}{L \text{ solution}} \qquad molality = m = \frac{moles \text{ solute}}{kg \text{ solvent}} \qquad \% \text{ mass} = \frac{mass \text{ solute}}{mass \text{ of solution}} \times 100$ $\% \text{ volume} = \frac{\text{vol of solute}}{\text{vol of solution}} \times 100 \qquad mole \text{ fraction} = \frac{moles \text{ of solute}}{t \text{ otal } \# \text{ of moles}}$ $parts \text{ per million} = ppm = \frac{g \text{ solute}}{g \text{ solution}} \times 10^6 = \frac{g \text{ solute}}{mL \text{ solution}} \times 10^6 \text{ when density}_{H2O} \text{: } 1.0 \text{ g/mL})$

mass of solution = mass of solvent + mass of solute

Kinetics

Property	Oth Order	1st Order	2nd Order
Rate Law	Rate = k	Rate = k[A]	$Rate = k[A]^2$
Units of k	mol L^{-1} s $^{-1}$	s^{-1}	$L mol^{-1} s^{-1}$
Integrated Rate Law	$[A]_t = -k \; t + [A]_0$	$ln[A]_t = -k \ t + ln[A]_0$	$\frac{1}{[A]_t} = k t + \frac{1}{[A]_0}$
Y vs × Plot	$[A]_t$ vs t	$\ln [A]_t$ vs. t	$\frac{1}{[A]_t}$ vs t
Slope, Y-intercept	-k, [A] ₀	-k, In [A] ₀	k, $\frac{1}{[A_0]}$
$Half\text{-}Life = t_{1/2}$	$\frac{[A]_0}{2 k}$	$\frac{0.693}{k}$	$\frac{\frac{1}{1}}{k \ [A]_0}$

1st-Order Decay: $N(t) = N_0 \exp(-k t)$

Integrated Form: $\ln N(t) = -k t + \ln (N_0)$

where: Rate Constant = k =
$$rac{0.693}{ au_{1/2}}$$
 and $au_{1/2}$ is the half-life

The Arrhenius equation relates the rate constant, k, to the activation energy, E_a at temperature T.

k = A e^{-E_a/RT}
$$\ln \frac{k_2}{k_1} = \frac{-E_a}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}, \text{ T in Kelvin, } \Delta \text{H in Joules.}$$

Equilibrium

The law of mass action exclude solids and pure liquids from the equilibrium expression.

$$\mathsf{aA} + \mathsf{bB} \longrightarrow \mathsf{cC} + \mathsf{dD} \qquad \mathsf{K}_c = \frac{[C]^c [D]^d}{[B]^b [A]^a} \qquad \mathsf{K}_p = \frac{(P_C)^c (P_D)^d}{(P_B)^b (P_A)^a}$$

The Equilbrium Constants: K_c and K_p Are Related

 ${\sf K}_p={\sf K}_c~~({\sf RT})^{\Delta n}~(\Delta{\sf n}=\#~{\sf moles}~{\sf of}~{\sf products}$ - $\#~{\sf moles}~{\sf of}~{\sf reactants})~{\sf R}=0.0821~{\sf L}~{\sf atm}~{\sf mol}^{-1}~{\sf K}^{-1}$

The van't Hoff equation relates K_1 at T_1 to K_2 at T_2

$$\ln \frac{K_2}{K_1} = \frac{-\Delta H_{rxn}^\circ}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \qquad \mathsf{R} = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}, \text{ T in Kelvin.}$$

Acids and Bases

 K_a (K_b) is the equilibrium constant for acids (bases).

$$\begin{aligned} \mathsf{HA} + \mathsf{H}_2\mathsf{O} &\longleftrightarrow \mathsf{H}_3\mathsf{O}^+ + \mathsf{A}^- & \mathsf{B} + \mathsf{H}_2\mathsf{O} &\longleftrightarrow \mathsf{B}\mathsf{H}^+ + \mathsf{O}\mathsf{H}^- \\ \mathsf{K}_a &= \frac{[\mathsf{H}^+][\mathsf{A}^-]}{[\mathsf{HA}]} & \mathsf{K}_b &= \frac{[\mathsf{O}\mathsf{H}^-][\mathsf{B}\mathsf{H}^+]}{[\mathsf{B}]} \end{aligned}$$

pH is a logarithmic measure of [H⁺]

 $pH = -log \ [H^+] \qquad pOH = -log \ [OH^-]$

The Ion-Product of Water is a constant for an aqueous system at 25°C.

 $K_w = [H^+] [OH^-] = 1.0 \times 10^{-14}$ and log form: pH + pOH = 14

Acid-Conjugate Base Dissociation Constants Are Related through the Ion-Product of Water.

$$\mathsf{K}_a \times \mathsf{K}_b = \mathsf{K}_w = 1.0 \times 10^{-14}$$
 or $\mathsf{pK}_a + \mathsf{pK}_b = 14$.

% Ionization of An Acid or a Base Is Found from equilibrium pH data.

% Ionization =
$$\frac{[\mathrm{H}^+]_{eq}}{[\mathrm{HI}]_{initial}} \times 100$$
 % Ionization = $\frac{[\mathrm{OH}^-]_{eq}}{[\mathrm{B}]_{initial}} \times 100$

ICE equiibrium problems simplify when K_a \times 100 < [HA] or when K_b \times 100 < [B]. The quadratic equation must be used when simplications can not be made.

$$ax^{2} + bx + c = 0$$
 $x = \frac{-b \pm \sqrt{b^{2} - 4ac}}{2a}$

The Henderson-Hasslebalch Equation is used to produce buffers.

$$\begin{aligned} \mathsf{HA} + \mathsf{H}_2\mathsf{O} &\longleftrightarrow \mathsf{H}_3\mathsf{O}^+ + \mathsf{A}^- & \mathsf{B} + \mathsf{H}_2\mathsf{O} &\longleftrightarrow \mathsf{BH}^+ + \mathsf{OH}^- \\ \mathsf{pH} &= \mathsf{pK}_a + \log \frac{[\mathsf{A}^-]_{init}}{[\mathsf{HA}]_{init}} & \mathsf{pOH} &= \mathsf{pK}_b + \log \frac{[\mathsf{BH}^+]_{init}}{[\mathsf{B}]_{init}} \end{aligned}$$

Thermodynamics

2nd Law of Thermodynamics: the entropy of the universe increases in all spontaneous processes.

$$\Delta S_{universe} = \Delta S_{system} + \Delta S_{surroundings} \qquad \Delta G_{rxn}^{\circ} = \Delta H_{rxn}^{\circ} - T\Delta S_{rxn}^{\circ}$$

The standard Gibb's Free Energy, $\Delta \mathbf{G}_{rxn}^{\circ}$ is used to predict the spontaneity of a reaction.

The cross-over temperature with which a spontaneous may be forced to occur can be calculated.

$$T > \frac{\Delta H_{rxn}^{\circ}}{\Delta S_{rxn}^{\circ}}$$
 (T in Kelvin, S and H have the same units J or kJ).

Under standard-state conditions, Hess's Law can be used to calculate thermodynamic quantities.

 $\mathsf{S}_{rxn}^{\circ} = \sum \mathsf{n}_i \mathsf{S}_{if}^{\circ}(\mathsf{products}) - \sum \mathsf{m}_j \mathsf{S}_{jf}^{\circ}(\mathsf{reactants}) \qquad \Delta \mathsf{H}_{rxn}^{\circ} = \sum \mathsf{n}_i \Delta \mathsf{H}_{if}^{\circ}(\mathsf{products}) - \sum \mathsf{m}_j \Delta \mathsf{H}_{jf}^{\circ}(\mathsf{reactants})$ $\Delta \mathsf{G}_{rxn}^{\circ} = \sum \mathsf{n}_i \Delta \mathsf{G}_{if}^{\circ}(\mathsf{products}) - \sum \mathsf{m}_j \Delta \mathsf{G}_{jf}^{\circ}(\mathsf{reactants})$ $\Delta \mathsf{G}_{nm}^{\circ} = \Delta \mathsf{H}_{--}^{\circ} - \mathsf{T} \Delta \mathsf{S}^{\circ} \qquad (\mathsf{T} \text{ in } \mathsf{K})$

$$\Delta {\sf G}_{rxn}^\circ = \Delta {\sf H}_{rxn}^\circ$$
 - T $\Delta {\sf S}_{rxn}^\circ$ (T in Kelvin, S and H in kJ)

 $\Delta \mathbf{G}_{rxn}$, can be calculated for reactions under non-standard state conditions.

$$\Delta {\sf G}_{rxn} = \Delta {\sf G}_{rxn}^\circ + RT \ln {\sf Q}$$
 ${\sf R} = 8.314$ J mol $^{-1}$ K $^{-1}$ and T in Kelvin)

 $\Delta \mathbf{G}_{rnx}^{\circ}$ is linked to the equilibrium constant, K, of a chemical reaction.

$$\Delta G_{rxn}^{\circ} = - RT \ln K_p \qquad \mathsf{R} = 8.314 \text{ Jmol}^{-1} \text{ K}^{-1} \text{ and T in Kelvin}$$
$$\mathsf{K} = \exp\left(\frac{-\Delta G_{rxn}^{\circ}}{RT}\right) \qquad (\mathsf{R} = 8.314 \text{ Jmol}^{-1} \text{ K}^{-1} \text{ and T in Kelvin})$$