## Chem 7/11 Equations In ATEX

## Stoichiometry \& Aqueous Solutions

The mole counts numbers of atoms or molecules using mass.
1 mole $=$ A.N. $=6.02 \times 10^{23}$ entitities $\quad \mathrm{MolX}=\frac{\operatorname{grams~} X}{\text { Molar Mass X }}$
$\%$ Yield $=\frac{\text { experimental mass }}{\text { theoretical mass }} \times 100$
\% Mass $\leftrightarrow$ Chemical Formula
$\%$ mass of Element $\mathrm{X}=\frac{\text { mol } X \text { in formula } \times \text { molar mass } / 1 \mathrm{~mol} \mathrm{X}}{\text { mass of } 1 \text { mol compound }}$
Molarity is a common concentration unit in aqueous chemistry. The dilution equation is used for the preparation of solutions using stock solutions.
molarity $=\mathrm{M}=\frac{\text { moles solute }}{\mathrm{L} \text { solution }} \quad M_{1} V_{1}=M_{2} V_{2}$

## Gases

The ideal gas law describes the behavior of gases at low pressure and high temperatures.
$P V=n R T \quad \frac{P_{1} V_{1}}{n_{1} T_{1}}=\frac{P_{2} V_{2}}{n_{2} T_{2}}$ (move constants to one side variables to another)
The gas law can be expressed as a function of molar mass and gas density.
MolarMass $=\frac{m R T}{V P}=\frac{d R T}{P} \quad 0.0821 \mathrm{~L} \mathrm{~atm} / \mathrm{mol} \mathrm{K}$ and T in Kelvin
Dalton's Law: $\mathbf{P}_{\text {Total }}$ of a mixture of gases is the sum of the partial pressures.
$P_{\text {total }}=\mathrm{P}_{1}+\mathrm{P}_{2}+\mathrm{P}_{3}+\ldots$.

## Thermochemistry

Internal and energy and enthalpy are state functions
$\Delta \mathrm{E}=q+w=q-P \Delta V \quad \Delta H=q_{p}=\Delta E+P \Delta V \quad \Delta \mathrm{H}_{r x n}^{\circ}=\Delta \mathrm{H}_{\text {products }}^{\circ}-\Delta \mathrm{H}_{\text {reactants }}^{\circ}$
Standard State is a specified experimental conditions of 1 atm ideal gas, 1 M liquids and 298 K .
Hess' Law and $\Delta \mathbf{H}_{f}^{\circ}$ values allows computation of $\Delta \mathbf{H}_{r x n}^{\circ}$ standard state conditions.
$\sum \mathrm{n}_{i} \Delta \mathrm{H}_{i f}^{\circ}$ (products) $-\sum \mathrm{m}_{j} \Delta \mathrm{H}_{j f}^{\circ}($ reactants $)$

## Quantum Theory

Energy is quantized at the molecular level. The speed of light in a vacuum is constant.
$E=h \nu \quad \mathrm{~h}=6.63 \times 10^{-34} \mathrm{~J} \mathrm{sec} \quad c=\lambda \nu=3.0 \times 10^{8} \mathrm{~m} / \mathrm{s}$

## 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 $\times \Delta T \quad$ OR $\quad q=\#$ Moles $\times$ Molar heat capacity $\times \Delta T$

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

$$
\mathrm{q}=\# \text { Moles } \times \Delta \mathrm{H}_{\text {fusion }} \text { and } \mathrm{q}=\# \text { Moles } \times \Delta \mathrm{H}_{\text {vaporization }}
$$

When calculating heat changes in matter the conservation of energy is obeyed.
$\sum q_{i}=q_{\text {heating solid }}+q_{\text {melting solid }}+q_{\text {heating liquid }}+q_{\text {vaporizing liquid }}+q_{\text {heating gas }}$
The Clausius-Clayperon relates the vapor pressure $\mathbf{P}_{1}$ at $\mathbf{T}_{1}$ to the vapor pressure $\mathbf{P}_{2}$ at $\mathbf{T}_{2}$.
$\ln \frac{P_{2}}{P_{1}}=\frac{-\Delta H_{\text {vap }}}{R}\left(\frac{1}{T_{2}}-\frac{1}{T_{1}}\right) \quad$ where R is $8.314 \mathrm{~J} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}$.
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.
$S=k_{\text {Henry }} \times P_{i}$
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.
$P_{\text {vapor }}=\chi_{\text {solvent }} P_{\text {solvent }}^{\circ}$
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 |
| :--- | :---: | :---: | :---: |
| $\Delta T_{b}=\left(T_{b}-T_{b}^{\circ}\right)=m \mathrm{~K}_{b}$ | $\Delta T_{f}=-\left(T_{f}-T_{f}^{\circ}\right)=m \mathrm{~K}_{f}$ | $\Delta \mathrm{P}_{\text {vapor }}=\chi_{\text {solute }} \mathrm{P}_{\text {solvent }}^{\circ}$ | $\pi=M R T$ |

## Concentration Units

Chemistry uses many units to specify concentration.

$$
\begin{aligned}
& \text { molarity }=\mathrm{M}=\frac{\text { moles solute }}{\mathrm{L} \text { solution }} \quad \text { molality }=\mathrm{m}=\frac{\text { moles solute }}{\mathrm{kg} \text { solvent }} \quad \% \text { mass }=\frac{\text { mass solute }}{\text { mass of solution }} \times 100 \\
& \% \text { volume }=\frac{\text { vol of solute }}{\text { vol of solution }} \times 100 \quad \text { mole fraction }=\frac{\text { moles of solute }}{\text { total } \# \text { of moles }} \\
& \text { parts per million } \left.=p p m=\frac{\mathrm{g} \text { solute }}{\mathrm{g} \text { solution }} \times 10^{6}=\frac{\mathrm{g} \text { solute }}{\mathrm{mL} \text { solution }} \times 10^{6} \text { when density }{ }_{H 2 O}: 1.0 \mathrm{~g} / \mathrm{mL}\right) \\
& \text { mass of solution }=\text { mass of solvent }+ \text { mass of solute }
\end{aligned}
$$

## Kinetics

| Property | Oth Order | 1st Order | 2nd Order |
| :--- | :--- | :--- | :--- |
| Rate Law | Rate $=\mathrm{k}$ | Rate $=\mathrm{k}[\mathrm{A}]$ | Rate $=\mathrm{k}[\mathrm{A}]^{2}$ |
| Units of k | mol L |  |  |
| Integrated Rate Law | $[\mathrm{A}]_{\mathrm{t}}=-\mathrm{kt}+[\mathrm{A}]_{0}$ | $\ln [\mathrm{~A}]_{\mathrm{t}}=-\mathrm{kt}+\ln [\mathrm{A}]_{0}$ | $\frac{\mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}}{[\mathrm{~A}]_{\mathrm{t}}}=\mathrm{kt}+\frac{1}{[\mathrm{~A}]_{0}}$ |
| Y vs $\times$ Plot | $[\mathrm{A}]_{t}$ vs t | $\ln [\mathrm{A}]_{t}$ vs. t | $\frac{1}{[A]_{t}} \mathrm{vs} \mathrm{t}$ |
| Slope, Y-intercept | $-\mathrm{k},[\mathrm{A}]_{0}$ | $-\mathrm{k}, \ln [\mathrm{A}]_{0}$ | $\mathrm{k}, \frac{1}{\left[A_{0}\right]}$ |
| Half-Life $=\mathrm{t}_{1 / 2}$ | $\frac{[A]_{0}}{2 k}$ | $\frac{0.693}{k}$ | $\frac{1}{k[A]_{0}}$ |

1st-Order Decay: $N(t)=N_{0} \exp (-k t) \quad$ Integrated Form: $\ln N(t)=-k t+\ln \left(N_{0}\right)$ where: Rate Constant $=\mathrm{k}=\frac{0.693}{\tau_{1 / 2}}$ and $\tau_{1 / 2}$ is the half-life

The Arrhenius equation relates the rate constant, $k$, to the activation energy, $\mathrm{E}_{a}$ at temperature T.
$\mathrm{k}=\mathrm{A} \mathrm{e}^{-E_{a} / R T} \quad \ln \frac{k_{2}}{k_{1}}=\frac{-E_{a}}{R}\left(\frac{1}{T_{2}}-\frac{1}{T_{1}}\right) \mathrm{R}=8.314 \mathrm{~J} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}, \mathrm{~T}$ in Kelvin, $\Delta \mathrm{H}$ in Joules.

## Equilibrium

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

$$
\mathrm{aA}+\mathrm{bB} \longrightarrow \mathrm{cC}+\mathrm{dD} \quad \mathrm{~K}_{c}=\frac{[C]^{c}[D]^{d}}{[B]^{b}[A]^{a}} \quad \mathrm{~K}_{p}=\frac{\left(P_{C}\right)^{c}\left(P_{D}\right)^{d}}{\left(P_{B}\right)^{b}\left(P_{A}\right)^{a}}
$$

The Equilbrium Constants: $K_{c}$ and $K_{p}$ Are Related
$\mathrm{K}_{p}=\mathrm{K}_{c}(\mathrm{RT})^{\Delta n}\left(\Delta \mathrm{n}=\#\right.$ moles of products - \# moles of reactants) $\mathrm{R}=0.0821 \mathrm{~L}$ atm mol ${ }^{-1} \mathrm{~K}^{-1}$
The van't Hoff equation relates $\mathrm{K}_{1}$ at $\mathrm{T}_{1}$ to $\mathrm{K}_{2}$ at $\mathrm{T}_{2}$
$\ln \frac{K_{2}}{K_{1}}=\frac{-\Delta H_{r x n}^{\circ}}{R}\left(\frac{1}{T_{2}}-\frac{1}{T_{1}}\right) \quad \mathrm{R}=8.314 \mathrm{~J} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}, \mathrm{~T}$ in Kelvin.

## Acids and Bases

$\mathrm{K}_{a}\left(\mathrm{~K}_{b}\right)$ is the equilibrium constant for acids (bases).

$$
\begin{array}{cl}
\mathrm{HA}+\mathrm{H}_{2} \mathrm{O} \longleftrightarrow \mathrm{H}_{3} \mathrm{O}^{+}+\mathrm{A}^{-} & \mathrm{B}+\mathrm{H}_{2} \mathrm{O} \longleftrightarrow \mathrm{BH}^{+}+\mathrm{OH}^{-} \\
\mathrm{K}_{a}=\frac{\left[\mathrm{H}^{+}\right]\left[\mathrm{A}^{-}\right]}{[\mathrm{HA}]} & \mathrm{K}_{b}=\frac{\left[\mathrm{OH}^{-}\right]\left[\mathrm{BH}^{+}\right]}{[\mathrm{B}]}
\end{array}
$$

pH is a logarithmic measure of $\left[\mathrm{H}^{+}\right]$
$\mathrm{pH}=-\log \left[\mathrm{H}^{+}\right] \quad \mathrm{pOH}=-\log \left[\mathrm{OH}^{-}\right]$

The lon-Product of Water is a constant for an aqueous system at $25^{\circ} \mathrm{C}$.
$\mathrm{K}_{w}=\left[\mathrm{H}^{+}\right]\left[\mathrm{OH}^{-}\right]=1.0 \times 10^{-14}$ and log form: $\mathrm{pH}+\mathrm{pOH}=14$
Acid-Conjugate Base Dissociation Constants Are Related through the Ion-Product of Water.
$\mathrm{K}_{a} \times \mathrm{K}_{b}=\mathrm{K}_{w}=1.0 \times 10^{-14} \quad$ or $\quad \mathrm{pK}_{a}+\mathrm{pK}_{b}=14$.
\% Ionization of An Acid or a Base Is Found from equilibrium pH data.

$$
\% \text { Ionization }=\frac{\left[\mathrm{H}^{+}\right]_{e q}}{[\mathrm{HI}]_{\text {initial }}} \times 100 \quad \% \text { lonization }=\frac{\left[\mathrm{OH}^{-}\right]_{e q}}{[\mathrm{~B}]_{\text {initial }}} \times 100
$$

ICE equiibrium problems simplify when $\mathrm{K}_{a} \times 100<$ [HA] or when $\mathrm{K}_{b} \times 100<$ [B]. The quadratic equation must be used when simplications can not be made.
$a x^{2}+b x+c=0 \quad \mathrm{x}=\frac{-b \pm \sqrt{b^{2}-4 a c}}{2 a}$
The Henderson-Hasslebalch Equation is used to produce buffers.

$$
\begin{array}{rr}
\mathrm{HA}+\mathrm{H}_{2} \mathrm{O} \longleftrightarrow \mathrm{H}_{3} \mathrm{O}^{+}+\mathrm{A}^{-} & \mathrm{B}+\mathrm{H}_{2} \mathrm{O} \longleftrightarrow \mathrm{BH}^{+}+\mathrm{OH}^{-} \\
\mathrm{pH}=\mathrm{pK}_{a}+\log \frac{\left[\mathrm{A}^{-}\right]_{\text {init }}}{[\mathrm{HA}]_{\text {init }}} & \mathrm{pOH}=\mathrm{pK}_{b}+\log \frac{\left[\mathrm{BH}^{+}\right]_{\text {init }}}{[\mathrm{B}]_{\text {init }}}
\end{array}
$$

## Thermodynamics

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

$$
\Delta \mathrm{S}_{\text {universe }}=\Delta \mathrm{S}_{\text {system }}+\Delta \mathrm{S}_{\text {surroundings }} \quad \Delta \mathrm{G}_{r x n}^{\circ}=\Delta \mathrm{H}_{r x n}^{\circ}-\mathrm{T} \Delta \mathrm{~S}_{r x n}^{\circ}
$$

The standard Gibb's Free Energy, $\Delta \mathbf{G}_{r x n}^{\circ}$ 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.

$$
\left.\mathrm{T}>\frac{\Delta H_{r x n}^{\circ}}{\Delta S_{r x n}^{\circ}} \quad \text { ( } \mathrm{T} \text { in Kelvin, } \mathrm{S} \text { and } \mathrm{H} \text { have the same units } \mathrm{J} \text { or } \mathrm{kJ}\right) \text {. }
$$

Under standard-state conditions, Hess's Law can be used to calculate thermodynamic quantities.
$\mathrm{S}_{r x n}^{\circ}=\sum \mathrm{n}_{i} \mathrm{~S}_{i f}^{\circ}$ (products) $-\sum \mathrm{m}_{j} \mathrm{~S}_{j f}^{\circ}$ (reactants) $\quad \Delta \mathrm{H}_{r x n}^{\circ}=\sum \mathrm{n}_{i} \Delta \mathrm{H}_{i f}^{\circ}$ (products) $-\sum \mathrm{m}_{j} \Delta \mathrm{H}_{j f}^{\circ}$ (reactants)
$\Delta \mathrm{G}_{r x n}^{\circ}=\sum \mathrm{n}_{i} \Delta \mathrm{G}_{i f}^{\circ}$ (products) $-\sum \mathrm{m}_{j} \Delta \mathrm{G}_{j f}^{\circ}$ (reactants)
$\Delta \mathrm{G}_{r x n}^{\circ}=\Delta \mathrm{H}_{r x n}^{\circ}-\mathrm{T} \Delta \mathrm{S}_{r x n}^{\circ} \quad(\mathrm{T}$ in Kelvin, S and H in kJ$)$
$\Delta \mathbf{G}_{r x n}$, can be calculated for reactions under non-standard state conditions.
$\Delta \mathrm{G}_{r x n}=\Delta \mathrm{G}_{r x n}^{\circ}+R T \ln \mathrm{Q} \quad \mathrm{R}=8.314 \mathrm{Jmol}^{-1} \mathrm{~K}^{-1}$ and T in Kelvin)
$\Delta \mathbf{G}_{r n x}^{\circ}$ is linked to the equilibrium constant, K , of a chemical reaction.
$\Delta \mathrm{G}_{r x n}^{\circ}=-R T \ln K_{p} \quad \mathrm{R}=8.314 \mathrm{~J} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}$ and T in Kelvin
$\mathrm{K}=\exp \left(\frac{-\Delta G_{r x n}^{\circ}}{R T}\right) \quad\left(\mathrm{R}=8.314 \mathrm{~J} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}\right.$ and T in Kelvin $)$

