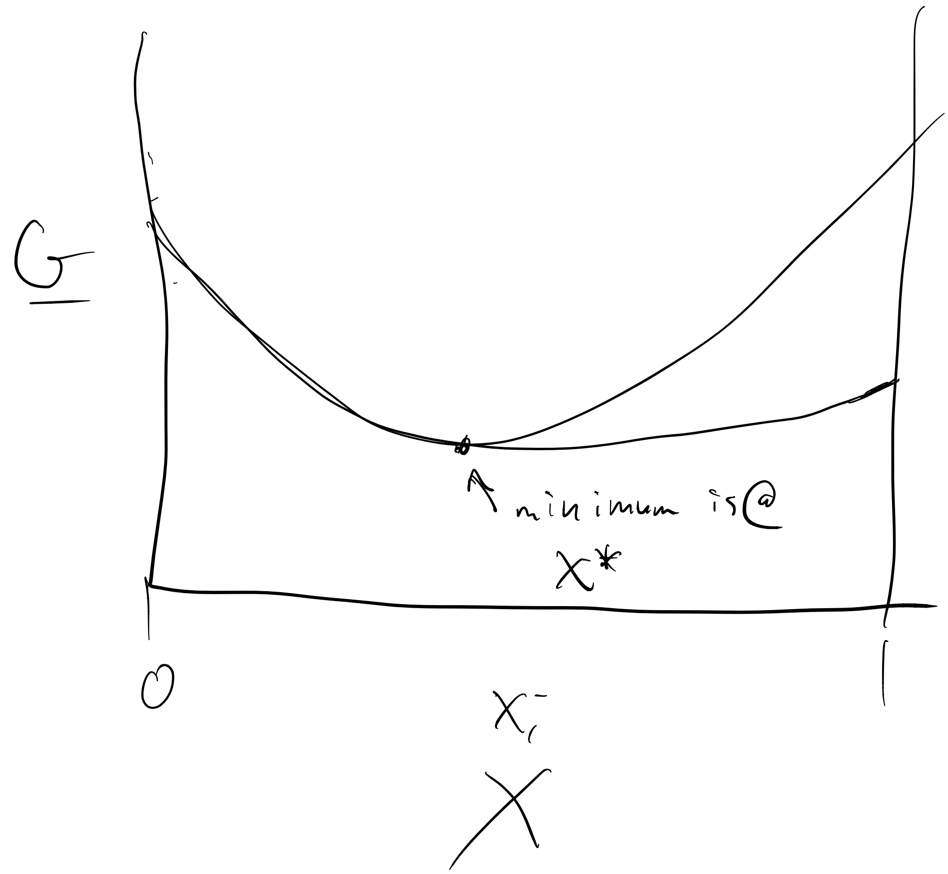
$$\ln\left(\prod x_i^{\nu_i}\right) = -\frac{\sum \nu_i \underline{G}_i}{RT}$$



System @ constant T, P evolves towards minimization of Gibbs Free energy

$$\underbrace{\prod_i x_i^{\nu_i}} < \exp\left[-\frac{\sum_i \nu_i \underline{G}_i(T,P)}{RT}\right]$$

we are to left of χ^*

reactants will be consumed and system will move towards χ^*

$$\prod x_i^{\nu_i} > \exp\left[-\frac{\sum_i \nu_i \underline{G}_i(T,P)}{RT}\right]$$

Then you are to the right of χ^* and system evolves to χ^* by consuming products $\rightarrow$ reactants

evolve to
$\rightarrow$

$$\rightarrow \prod x_i^{\nu} = \exp\left[-\frac{\sum_i \nu_i \underline{G}_i(T,P)}{RT}\right]$$

Since chemical RXNs can proceed in either direction → they are called <u>Reversible</u>

A chemical RXN goes to completion if it proceeds until one of the reactants is <u>completely consumed</u>.

this <u>never</u> happens "completely" but for practical purposes it can be thought of that way

$$H_2 + \underline{\underline{\tfrac{1}{2}}} O_2 = H_2O$$

$$\frac{\Delta G_{rxn}}{RT} = \frac{-228570 \text{ J/mol}}{8.314 \text{ J/(mol K)} \cdot 298.15 \text{ K}} = -92.21$$

Species	Initial moles	Final moles	Mole fraction
H_2	1	$1-X$	$(1-X)/(1.5-0.5X)$
O_2	0.5	$0.5-0.5\cdot X$	$0.5(1-X)/(1.5-0.5X)$
H_2O	0	X	$X/(1.5-0.5X)$
Total	1.5	$1.5-0.5X$	1

<u>What is X?</u>

$$\exp\left(-\frac{\sum \nu_i G_i}{RT}\right) = \prod x_i^{\nu_i}$$

$$\exp(-(-92.21)) \simeq 1.11 \cdot 10^{40}$$

$$\frac{x_{H_2O}}{x_{H_2} x_{O_2}^{0.5}} = \frac{x(1.5-0.5x)^{0.5}}{0.5^{0.5}(1.0-x)^{1.5}}$$

$$x \approx 1.0 - 3 \cdot 10^{-27} \approx 1$$

how do you estimate $\Delta_{rxn} G$?

$$x_{H_2O}^{1} \cdot x_{H_2}^{-1} \cdot x_{O_2}^{-0.5}$$

→ one possible starting point is to rewrite the G w/ a standard state G and a deviation away from the standard state G.

→ need to choose T, P, and x_i^0

convenient T ~ 25°C

G_i standard state { P ~ 1 bar; x_i^0 → bring x_i to 1 } many steps

Equilibrium constant

$$K_a(T) = \exp\left(\frac{-\Delta_{rxn} G^\circ}{RT}\right)$$

$$\boxed{\Delta_{rxn} G^\circ(T = 25^\circ C) = \sum_i r_i \Delta_f \underline{G}_i^\circ (T=25^\circ C)}$$

$\Delta_f \underline{G}^\circ$ is the standard Gibb's free energy of formation

You can find and calculate these

Recall - energy balances here

H! enthalpy - not $\underline{G}$

how does H relate to G?

$$G = H + PV$$

$$G(T) = H(T) + PV$$

Goal → get rid of $\underline{G}$
so we can couple RxNs directly
to our energy balance equations

⋮

$$\left.\frac{d \ln K_a}{dT}\right|_P = -\frac{1}{R}\frac{d}{dT}\left[\frac{\sum r_i \Delta_f \underline{G}_i}{T}\right]$$

$$= \frac{1}{RT^2}\sum r_i \Delta_f \underline{H}_i^\circ = \frac{\Delta_{rxn} H^\circ(\underline{T})}{RT^2}$$

find these or calculate.

$$\boxed{\Delta_{rxn} H^\circ (T = 25^\circ C) = \sum_i \nu_i \Delta_f H_i^\circ (T = 25^\circ C)}$$

find these

$$\boxed{\ln\left[\frac{K_a(T_2)}{K_a(T_1)}\right] = -\frac{\Delta_{rxn} H^\circ}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$$

$$\boxed{K_a(T_2) = K_a(T_1)\exp\left(-\frac{\Delta_{rxn} H^\circ}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right)}$$

Avg. ~ 73