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Course 565/665 Lecturer Prof. Cavagnero

Day 4.8.04 Date 9:55 am

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K as a function of Pressure

$$K = \frac{N_c^c}{N_A^a N_B^b} = \frac{\left(\frac{P_c V}{kT}\right)^c}{\left(\frac{P_A V}{kT}\right)^a \left(\frac{P_B V}{kT}\right)^b} = \frac{q_c^c}{q_A^a q_B^b} e^{-\Delta\varepsilon_0/kT}$$

$$K = \frac{P_c^c}{P_A^a P_B^b} = (kT)^{(c-a-b)} \frac{q_{0c}^c}{q_{0A}^a q_{0B}^b} e^{-\Delta\varepsilon_0/kT}$$

where $q_0 \equiv \frac{q}{V}$, $q_0' = \frac{q'}{V}$

$$\mu = -kT \ln\left(\frac{q'}{N}\right)$$

$$\mu = -kT \ln\left(\frac{q'}{N}\right) = -kT \ln\left(\frac{q_0' V}{N}\right) = -kT \ln\left(\frac{q_0' kT}{P}\right)$$

$$\begin{cases} P_0 \equiv q_0' kT \\ \mu_0 \equiv -kT \ln P_0 \end{cases}$$

standard chemical potential

$\mu_0 = \mu_0(T, q')$

usually standard states are defined at $T = 25°C$, specially for solvent.

$$\mu = \mu_0 + kT \ln P$$

Define $K \equiv K_p$.

1 of 2

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for chem. rxn.

$$\Delta\mu = \Delta\mu_0 + kT \ln \frac{P_C^c}{P_A^a P_B^b} = \Delta\mu_0 + kT \ln K_P$$

$$\Delta\mu = c\mu_C - a\mu_A - b\mu_B \; ; \quad \Delta\mu_0 = c\mu_{0C} - a\mu_{0A} - b\mu_{0B}$$

How do Rxns react a perturbation of equilibrium ? "Le Chatelier Principle"

$$A \rightleftharpoons B \qquad K_{AB}$$

at constant T. P. $dG = \mu_A dN_A + \mu_B dN_B$ $\quad dN_A = -dN_B \quad N_A + N_B = N$

$N_B \equiv N \cdot \xi$ (ξ : rxn progress parameter)

$dG = (\mu_B - \mu_A) N d\xi$

at eq. $dG = 0$; towards equilibrium $dG = (\mu_B - \mu_A) N d\xi < 0$

$\Rightarrow \mu_B - \mu_A$ and $d\xi$ has opposite sign.

if ① perturbation $\uparrow \mu_B$, then $\mu_B - \mu_A > 0$, $\Rightarrow d\xi < 0$ $\quad B \downarrow$

② perturbation $\downarrow \mu_B$. $\mu_B - \mu_A < 0$, $\Rightarrow d\xi > 0$ $\quad B \uparrow$.