

$$A(a_0) + B(a_0) \rightarrow P(a_0)$$



$$r_{AB} = r_A + r_B$$

$$j_B = -D_B \frac{dc_B}{dx}$$

$$j_A = \frac{1}{A} \frac{da_A}{dt} \quad j_{r,B} = -D_B \frac{dc_{B,r}}{dr}$$

$$j_{r,B} = \frac{1}{A} \frac{da_B}{dt} \Rightarrow \frac{da_B}{dt} = j_{r,B} A$$

$$\frac{da_B}{dt} = 4\pi r^2 j_{r,B} = 4\pi r^2 D_B \frac{dc_{B,r}}{dr}$$

$$A_B = -\frac{da_B}{dt} = 4\pi r^2 D_B \frac{dc_{B,r}}{dr}$$

$$A_B \frac{dr}{r^2} = 4\pi D_B dc_{B,r} \quad \int_{r_0}^r \frac{dr}{r^2} = 4\pi D_B \int_0^{c_0} dc_{B,r}$$

$$R_B \frac{1}{r_0} = 4\pi D_B c_0$$

$$-\frac{da_B}{dt} = 4\pi D_B c_0 r_{AB}$$

$$N_A = c_A V_L$$

$$-\frac{da_B}{dt} = 4\pi D_B r_{AB} V_L c_A c_0$$

$$D_{AB} = D_A + D_B$$

$$-\frac{da_B}{dt} = 4\pi D_{AB} r_{AB} V_L c_A c_0 \quad \left| \frac{1}{V} \right.$$

$$-\frac{da_B}{dt} \frac{1}{V} = \frac{dc_0}{dt} = v = \frac{4\pi D_{AB} r_{AB} L}{k} c_A c_0$$

$$v = k c_A c_0$$

$$k = 4\pi D_{AB} r_{AB} L$$

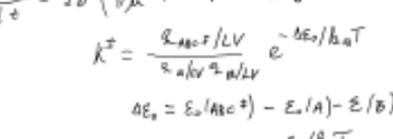
$$D_A = \frac{k_B T}{6\pi \eta r_A} \quad D_B = \frac{k_B T}{6\pi \eta r_B}$$

$$k = \frac{2}{3} r_{AB} \frac{k_B T}{\eta} L \left( \frac{1}{r_A} + \frac{1}{r_B} \right)$$

$$r_A = r_B = \frac{1}{2} r_{AB} \Rightarrow k = \frac{8}{3} \frac{RT}{\eta}$$

$$k = 4\pi r_{AB} D_{AB} \frac{f}{e^2 - 1}$$

$$f = \frac{2\epsilon_0 \epsilon_r c^2}{4\pi \epsilon_0 \epsilon_r k_B T r_{AB}}$$



$$v = \frac{dc_A}{dt} = \frac{d[ABC^\ddagger]}{dt} = k^\ddagger [ABC^\ddagger] = \frac{k^\ddagger K^\ddagger}{k} c_A c_B$$

$$K^\ddagger = \frac{c_{ABC^\ddagger}}{c_A c_B}$$

$$\frac{1}{2} \frac{dc_A}{dt} = \frac{1}{2} \frac{d[ABC^\ddagger]}{dt} = k^\ddagger c_A c_B$$

$$K^\ddagger = \frac{c_{ABC^\ddagger}}{c_A c_B} = \frac{c_{ABC^\ddagger} / V}{c_A / V \cdot c_B / V} = \frac{z_{ABC^\ddagger} / V}{z_A z_B} e^{-\epsilon_{ABC^\ddagger} / k_B T}$$

$$z = \frac{q}{\sigma} e^{-\epsilon / k_B T}$$

$$\frac{N_i}{N} = \frac{q_i e^{-\epsilon_i / k_B T}}{q}$$

$$\frac{N_i}{N} = \frac{q_i}{q} e^{-\epsilon_i / k_B T} \quad \Delta \epsilon = \epsilon_i - \epsilon_j$$

$$z = z_A \cdot z_B \cdot z_{C^\ddagger} \cdot z_e$$

$$z_{ABC^\ddagger} = q_A z_B z_{C^\ddagger} = z_A z_B z_{C^\ddagger} z_e$$

$$z_{C^\ddagger} = \frac{(2\pi \mu k_B T)^{3/2}}{h^3} \sigma$$

$$K = z_{ABC^\ddagger} K^\ddagger$$

$$\frac{dc_A}{dt} = \frac{1}{2} \frac{d[ABC^\ddagger]}{dt} = \frac{1}{2} \frac{d}{dt} \left( \frac{2 k_B T}{\pi \mu} \right)^{3/2} z_A z_B K^\ddagger c_A c_B$$

$$k = \frac{1}{2} \frac{d}{dt} \left( \frac{2 k_B T}{\pi \mu} \right)^{3/2} \frac{(2\pi \mu k_B T)^{3/2} \sigma}{h^3} c_A c_B$$

$$k = \frac{k_B T}{h} K^\ddagger \quad \text{EYRING}$$

$$k = \chi \frac{k_B T}{h} K^\ddagger$$

$$A + B \xrightarrow{K^\ddagger} ABC^\ddagger \xrightarrow{k^\ddagger} P$$

$$K^\ddagger \approx K^\ddagger = \frac{c_{ABC^\ddagger}}{c_A c_B}$$

$$K^\ddagger = \frac{z_{ABC^\ddagger}}{z_A z_B} = \frac{z_A z_B z_{C^\ddagger} z_e}{z_A z_B} = z_{C^\ddagger} z_e$$

$$k = \frac{k_B T}{h} K^\ddagger = \frac{k_B T}{h} z_{C^\ddagger} z_e$$

$$\Delta^\ddagger G = -RT \ln K^\ddagger$$

$$\Delta^\ddagger G = \Delta^\ddagger H^\ddagger - T \Delta^\ddagger S^\ddagger$$

$$(g) \quad k = \frac{k_B T}{h} \left( \frac{RT}{V^\ddagger} \right)^{m-1} K^\ddagger$$

$$(2b) \quad k = \frac{k_B T}{h} \left( \frac{1}{\sigma} \right)^{m-1} K^\ddagger$$

$$k = \frac{k_B T}{h} \left( \frac{RT}{V^\ddagger} \right)^{m-1} e^{-\Delta^\ddagger H^\ddagger / RT} e^{\Delta^\ddagger S^\ddagger / R}$$

$$k = \frac{k_B T}{h} \left( \frac{1}{\sigma} \right)^{m-1} e^{-\Delta^\ddagger H^\ddagger / RT} e^{\Delta^\ddagger S^\ddagger / R}$$

$$k = A e^{-E_a / RT} \quad k = k^\ddagger K^\ddagger$$

$$E_a = RT^2 \frac{d \ln k}{dT}$$

$$\frac{d \ln k}{dT} = \frac{mRT + \Delta^\ddagger H^\ddagger}{RT^2}$$

$$(g) \quad E_a = \Delta^\ddagger H^\ddagger + mRT$$

$$(2b) \quad E_a = \Delta^\ddagger H^\ddagger + RT$$

$$(2b) \quad k = \frac{k_B T}{h} \left( \frac{1}{\sigma} \right)^{m-1} e^{-E_a / RT} e^{\Delta^\ddagger S^\ddagger / R}$$

$$(g) \quad A = \frac{k_B T}{h} \left( \frac{1}{\sigma} \right)^{m-1} e^{\Delta^\ddagger S^\ddagger / R}$$

$$\ln \frac{k}{T} = \ln \left( \frac{k_B}{h} \left( \frac{1}{\sigma} \right)^{m-1} \right) - \frac{\Delta^\ddagger H^\ddagger}{RT} + \frac{\Delta^\ddagger S^\ddagger}{R}$$



$$\Delta^\ddagger X = X_{AB^\ddagger} - X_{AB} - X_B$$

$$\Delta^\ddagger V = V_{AB^\ddagger} - V_A - V_B$$

$$k = \frac{k_B T}{h} \left( \frac{1}{\sigma} \right)^{m-1} e^{-\Delta^\ddagger G^\ddagger / RT}$$

$$dG = V dp - S dT$$

$$\left( \frac{\partial G}{\partial p} \right)_T = V \Rightarrow \left( \frac{\partial \Delta^\ddagger G^\ddagger}{\partial p} \right)_T = \Delta^\ddagger V$$

$$\ln k = \ln \left( \frac{k_B T}{h} \left( \frac{1}{\sigma} \right)^{m-1} \right) - \frac{\Delta^\ddagger G^\ddagger}{RT}$$

$$\left( \frac{\partial \ln k}{\partial p} \right)_T = -\frac{1}{RT} \left( \frac{\partial \Delta^\ddagger G^\ddagger}{\partial p} \right)_T$$

$$\left( \frac{\partial \ln k}{\partial p} \right)_T = -\frac{\Delta^\ddagger V}{RT}$$

$$\ln \frac{k}{k_0} = -\frac{\Delta^\ddagger V}{RT} \int_{p_0}^p dp$$

$$\ln \frac{k}{k_0} = -\frac{\Delta^\ddagger V}{RT} (p - p_0)$$

$$\ln k \quad \text{negativ} = -\frac{\Delta^\ddagger V}{RT}$$