Chem Dynamics Cheatsheet

Reaction Dynamics

$$k_R = A e^{-E_a/RT}$$

$$\sigma = \pi d^2$$

$$Z_{AB} = \sigma v_{rel} N_A^2 [A][B]$$

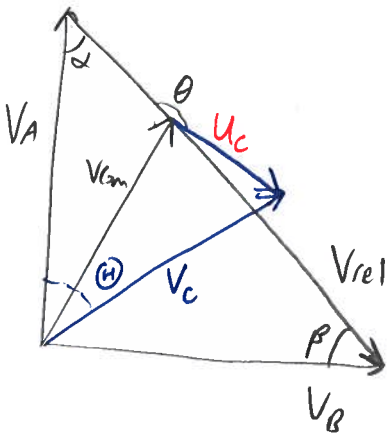
$$Z_{nA} = \frac{1}{2}\sigma v_{rel} N_A^2 [A]^2$$

$$v_{rel} = \sqrt{\frac{8kT}{\pi\mu}}$$

$$\sigma_R = P\sigma \;|\; \sigma_R = \pi R_c^2$$

$$k_R = P\sigma v_{rel} N_A e^{-E_a/RT}$$

$$R_c = \frac{e^2}{4\pi\varepsilon_0 E}$$



$$V_{com} = V_c - u_c$$

$$V_{rel} = V_B - V_A$$

$$m_A u_A + m_B u_B = 0$$

$$\frac{1}{2}m_A u_A^2 + \frac{1}{2}m_B u_B^2 = \mu\frac{1}{2}v_{rel}^2$$

$$V_{com} = V_A + \frac{m_B}{m_A+m_B}V_{rel}$$

$$\|u_B\| = \frac{m_B}{m_A+m_B}|V_{rel}|$$

Fick's First Law

$$J = -D_B \frac{\partial[B]}{\partial x}$$

Fick's 2nd Law

$$\frac{\partial[B]}{\partial t} = D_B \frac{\partial^2[B]}{\partial x^2}$$

$$k_d = 4\pi R^* D N_A$$

$$D_i = \frac{kT}{6\pi\eta R_i}$$

$$k_d = \frac{8RT}{3\eta}$$

$$J_{conv} = [B]_v$$

$$\frac{\partial[B]}{\partial t} = D_B\nabla^2[B] - v\nabla[B] - k_r[B]$$

LASERS

$$\underline{E} = \underline{A_0} e^{i(\omega t - k_2 z)}$$

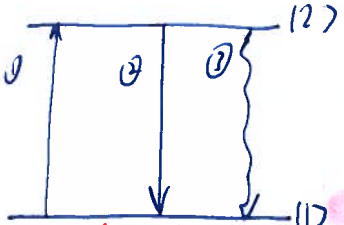
$$I = c\varepsilon_0 E_0^2$$

$$I \propto E_0^2$$

$$\rho(\nu,T)\,d\nu = \frac{8\pi h\nu^3}{c^3(e^{h\nu/kT}-1)}\,d\nu$$

$$A_{ik} = \frac{8\pi h\nu^3}{c^3}B_{ik}$$

$$B_{ik} = \frac{g_k}{g_i}B_{ki}$$



① : $-\frac{dN_1}{dt} = \frac{dN_2}{dt} = B_{12}\rho(\nu)N_1$

② : $-\frac{dN_2}{dt} = \frac{dN_1}{dt} = B_{21}\rho(\nu)N_2$

③ : $-\frac{dN_2}{dt} = \frac{dN_1}{dt} = A_{21}N_2$

$$I(\omega) = \frac{I(\omega_0)\Gamma_N^2}{(\omega_0-\omega)^2+\Gamma_N^2}$$

$$\Gamma_D = \omega_0\sqrt{\frac{8kT\ln 2}{mc^2}}$$

$$A_{ik} = \tau^{-1} = \Gamma_N$$

Pressure Broadening

$$\Gamma_c = \sqrt{\frac{8k_BT}{\pi\mu}}\,\sigma_{eff}\,C$$

$$C = \frac{N_A P}{RT}$$

Doppler Broadening

$$\omega_c = \omega\left(1 - \frac{v_z}{c}\right)$$

Gaussian Profile

$$I(\omega) = I(\omega_1)e^{-\left(\frac{c(\omega-\omega_0)}{\omega_0 v_p}\right)^2}$$

$$v_p = \sqrt{\frac{2kT}{m}}$$

$$\frac{\Gamma_D}{\omega_0} = \frac{1}{c}\sqrt{\frac{8kT\ln 2}{m}}$$

$$= 7.16\times10^{-7}\sqrt{\frac{T(K)}{M(u)}}$$ rad s^{-1}

Lasing:

Beer-Lambert Law

$$I = I_0 e^{-\alpha(\nu)cl}$$

Gain factor per round trip

$$G(\nu) = e^{-2\alpha(\nu)L}$$

Loss coeff: γ $\quad I = I_0 e^{-\gamma}$

Total intensity:

$$I(\nu, 2L) = I(\nu)\,e^{-2\alpha(\nu)L-\gamma}$$

Mode Locking pulse duration

$$\tau = \frac{a}{\Gamma}$$