

Constants and Formulas

$$R = 8.315 \text{ J K}^{-1} \text{ mol}^{-1} ; \quad 1 \text{ atm} = 101325 \text{ Pa} ; \quad N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$$

$$k_B = 1.381 \times 10^{-23} \text{ J K}^{-1} ; \quad h = 6.6261 \times 10^{-34} \text{ J s}$$

Half-life, $t_{1/2}$: time at which $[A] = [A]_0/2$

Integrated rate laws.

$$[A] = [A]_0 - kt ; \quad [A] = [A]_0 e^{-kt} ; \quad 1/[A] = 1/[A]_0 + 2kt$$

$$\ln \left(\frac{[B][A]_0}{[B]_0[A]} \right) = ([B]_0 - [A]_0)kt$$

$$A \rightarrow I \rightarrow P: \quad P = \left(1 - \frac{k_1 e^{-k_2 t} - k_2 e^{-k_1 t}}{k_1 - k_2} \right) [A]_0$$

$$A \rightleftharpoons P: \quad [A] = [A]_0 \frac{k_r + k_f e^{-kt}}{k}$$

T-jump experiment: $x = [A] - [A]_{eq,2} = x_0 \exp(-(k_{f2} + k_{r2})t)$

Arrhenius: $k = A e^{-E_a/RT}$

Eyring: $k = \kappa \frac{k_B T}{hc^\circ} e^{\Delta S^\ddagger/R} e^{-\Delta H^\ddagger/RT}$

For reactions in the gas phase ($z = 1$ or c°):

$$E_a = \Delta H^\ddagger + mRT$$

$$A = \frac{e^m k_B T}{hz} e^{\Delta S^\ddagger/R}$$

Diffusion constant:

$$k_d = 4\pi N_A (r_A + r_B) D_{AB} ; \quad D_{AB} = D_A + D_B ; \quad D_A = \frac{k_B T}{6\pi\eta r_A}$$

Lindemann mechanism:

$$R = k_{uni}[A] ; \quad k_{uni} = \frac{k_2 k_1 [M]}{k_{-1}[M] + k_2}$$

Michaelis-Menten mechanism, enzymatic reactions:

$$R_0 = \frac{k_2[E]_0[S]_0}{[S]_0 + K_m} = \frac{R_{max}[S]_0}{[S]_0 + K_m} ; \quad K_m = (k_{-1} + k_2)/k_1$$

Enzymatic reactions with competitive inhibition:

$$R_0 = \frac{k_2[E]_0[S]_0}{[S]_0 + K_m^*} ; \quad K_m^* = K_m(1 + [I]/K_i) ; \quad K_i = [E][I]/[EI]$$

Langmuir model of adsorption:

$$\theta = V_{adsorbed}/V_m = k_a P / (k_a P + k_d) = KP / (KP + 1)$$

Dissociative chemisorption of $A_2(g)$:

$$\theta = (KP)^{1/2} / (1 + (KP)^{1/2})$$

Chain-branching reactions:

$$[R\cdot] = (k_i[A][B]/k_{eff})(e^{-k_{eff}t} - 1) ; \quad k_{eff} = k_b(\phi - 1) - k_t$$

Beer-Lambert law:

$$I_{abs} = 2.303 I_0 \epsilon \ell [A]$$

Quantum yield:

$$\Phi_j = \frac{k_j}{k_1 + k_2 + k_3 + \dots} ; \quad k_f \tau_f = \Phi_f$$

Quenching:

$$R_q = k_q[S_1][Q] ; \quad I_f^0/I_f = 1 + (k_q/k_f)[Q]$$

FRET:

$$\Phi_{FRET} = \frac{1}{1 + (r/r_0)^6}$$

Electron transfer:

$$k_{e.t.} \propto e^{\beta r} e^{-\Delta G^\ddagger/RT} ; \quad \Delta G^\ddagger = (\Delta G^\circ + \lambda)^2/4\lambda$$