Richards

$$\% \, ee = \frac{R + S}{R - S} \; x \; 100$$

$$\% = \frac{\% \, ee + 100}{2}$$

$$[\alpha]_o = \frac{[\alpha]}{l \; x \; c} \; x \; 100$$

$$OP = \frac{[\alpha]}{[\alpha]_o} x \; 100 = ee \; (under \; ideal \; conditions)$$

$$\Delta\Delta G^{\ddagger} = -RTlnK$$

$$\frac{k_1}{k_2} = e^{-\frac{\Delta\Delta G^{\ddagger}}{RT}}$$

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

$$s = \frac{k_{fast}}{k_{slow}} = \frac{\ln(1-c)(1-ee_s)}{\ln(1-c)(1+ee_s)} \qquad ee_s = -ee_p$$

$$c = \frac{ee_s}{ee_s + ee_p} \; x \; 100$$

$$ACE = \frac{mR_{prod}}{mR_{cat}} x \frac{1}{mol\%} \; x \; \frac{\% \, ee}{100} \; x \; \%$$

Paz

$$\sigma_x = \log \frac{k_a(XC_6H_4COOH)}{k_a(C_6H_5COOH)} = pK_a(C_6H_5COOH) - pK_a(XC_6H_4COOH)$$

$$\log\left(\frac{k_x}{k_H}\right) = \rho\sigma$$

$$k = Ae^{-\frac{Ea}{RT}} \qquad lnk = -\frac{Ea}{RT} + lnA$$

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

In addition to this need to know rate equations and half-life equations.

Vasily

$$F_i = m_i a_i = -\frac{dE_i}{dr_i}$$

$$r(t+\delta t) = 2r(t) - r(t-\delta t) + \frac{F(t)}{m}\delta t^2$$

$$E_{total} = E_{bonded} + E_{non-bonded}$$

$$E_{bonded} = V_{bond} + V_{angle} + V_{torsion} + V_{constraint}$$

$$E_{non-bonded} = V_{qq} + V_{vdw} + V_{hb}$$

$$V_{bond} = \frac{K_r}{2}(r - r_o)^2$$

$$V_{angle} = \frac{K_\theta}{2}(\theta - \theta_o)^2$$

$$V_{torsion} = \frac{V_\phi}{2}[1 + \cos(n\phi - \gamma)]$$

$$V_{constraint} = \frac{K_\phi}{2}(\phi - \phi_o)^2$$

$$V_{qq} = \frac{q_i q_j}{r_{ij}} \frac{|e^2|}{4\pi\varepsilon_o\varepsilon}$$

$$V_{vdw} = \frac{A_{ij}}{r_{ij}^{12}} + \frac{B_{ij}}{r_{ij}^{6}}$$

$$V_{hb} = \frac{c_{ij}}{r_{ij}^{12}} + \frac{D_{ij}}{r_{ij}^{10}}$$

$$\Delta G = -RTln\left(\frac{P_2}{P_1}\right)$$

Meech

Transition State Theory

$$q_v = \frac{1}{1 - e^{-\frac{hv}{kT}}} \qquad q_{v\,(low\,T)} = 1 \qquad q_{v\,(high\,T)} = \frac{kT}{hv}$$

$$q_{R\,(linear)} = \frac{8\pi^2 IkT}{\sigma h^2} \qquad q_{R\,(non-linear)} = \left(\frac{kT}{hc}\right)^{\frac{3}{2}} \left(\frac{\pi}{ABC}\right)^{\frac{1}{2}}$$

$$q_{T\,(1D)} = \left(\frac{2\pi mkT}{h^2}\right)^{\frac{1}{2}} x \qquad q_{T\,(3D)} = (2\pi mkT)^{\frac{3}{2}} \frac{V}{h^3}$$

$$k_{TST} = \frac{kT}{h} \frac{q_R^{\ddagger} q_T^{\ddagger} q_{vV}}{q_{AB} q_C} e^{-\frac{E_o}{RT}}$$

$I = \mu r^2$ 3N-6 = non linear 3N-5 = linear

Transition State Theory in Solution

$$z = \sigma \bar{c}_{rel} N \qquad \sigma = \pi r^2 \qquad \bar{c}_{rel} = \left(\frac{8kT}{\pi m}\right)^{\frac{1}{2}} \qquad N = \frac{liquid\ density\ x\ N_A}{atomic\ mass}$$

$$k_{kramers} = \frac{\omega_r}{2\pi\omega_b}\left(\left(\frac{\gamma^2}{4} + \omega_b^2\right)^{\frac{1}{2}} \frac{\gamma}{2}\right) e^{-\frac{E_a}{kT}}$$

$$\gamma = \eta \qquad k_{kramers\,(\eta\to 0)} = \frac{\omega_r}{2\pi} e^{-\frac{Ea}{kT}} \qquad k_{kramers\,(\eta \gg \omega b)} = \frac{\omega_r \omega_b}{2\pi\eta} e^{-\frac{Ea}{kT}}$$

Need to know how to derive upper and lower limits

Electron Transfer Reactions

$$k_{ET} = 2 < H_{DA} >^2 \left(\frac{\pi^3}{4\pi RT}\right)^{\frac{1}{2}} e^{-\frac{\Delta G^{\ddagger}}{RT}}$$

$$< H_{DA} >^2 = < H_{DA}^o >^2 e^{-\beta r}$$

$$< H_{DA} > = \int \psi_o \hat{H}_{DA} \psi_A d\tau$$

$$G_i = G_i^o + \frac{1}{2}\omega s^2 (x - x_i)^2$$

$$x_c = \frac{1}{2}(x_A + x_D) + \frac{\Delta G^o}{\omega s^2 (x_A - x_D)}$$

$$\Delta G^{\ddagger} = \frac{1}{2}\omega s^2 \left(\frac{1}{2}(x_A - x_D) + \frac{\Delta G^o}{\omega s^2 (x_A - x_D)}\right)$$

$$\lambda = \frac{1}{2}\omega s^2 (x_D - x_A)^2$$

$$\Delta G^{\ddagger} = \frac{(\lambda + \Delta G^o)^2}{4\lambda}$$

$$lnk_{ET} = lnA - \frac{\Delta G^{\ddagger}}{RT} = constant - \frac{(\Delta G_o + \lambda)^2}{4\lambda RT}$$
$$= -\frac{\Delta G_o^2}{4RT\lambda} - \frac{\Delta G_o}{2RT} - \frac{\lambda}{4RT} + constant$$

$$\frac{\delta lnk_{ET}}{\delta \Delta G_o} = -\frac{\Delta G_o}{2\lambda RT} - \frac{1}{2RT} = 0 \qquad \Delta G_o = -\lambda$$