



$$\hat{H}\Psi = i\hbar \frac{\partial}{\partial t} \Psi$$

$$\lambda_s = \frac{(\Delta q)^2}{2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \left(\frac{1}{a} - \frac{1}{2d} \right)$$

$$E^\circ = -\frac{\Delta G^\circ}{nF}$$

$$\lambda_i = \frac{1}{2} [E_{\text{ox}}(R_{\text{eq}}^{\text{red}}) - E_{\text{ox}}(R_{\text{eq}}^{\text{ox}}) + E_{\text{red}}(R_{\text{eq}}^{\text{ox}}) - E_{\text{red}}(R_{\text{eq}}^{\text{red}})]$$

$$pK_a = \frac{\Delta G^\circ}{\ln(10)RT}$$

$$\Delta \tilde{U}_{\mu\nu} = \Delta U_{\mu\nu} + k_B T \ln(Q^{\text{II}}/Q^{\text{I}})$$

$$k^{\text{EPT}}(\eta) = \int P(R) k^{\text{EPT}}(\eta; R) dR$$

$$k_a^{\text{ET}}(\eta) = \frac{(V^{\text{el}})^2}{\beta' \hbar} \sqrt{\frac{\pi}{k_B T \lambda}} \rho_M \int d\epsilon [1 - f(\epsilon)] \exp \left[-\frac{(\epsilon - e\eta + \lambda)^2}{4\lambda k_B T} \right]$$

$$k_c^{\text{ET}}(\eta) = \frac{(V^{\text{el}})^2}{\beta' \hbar} \sqrt{\frac{\pi}{k_B T \lambda}} \rho_M \int d\epsilon f(\epsilon) \exp \left[-\frac{(-\epsilon + e\eta + \lambda)^2}{4\lambda k_B T} \right]$$

$$P(R) = \sqrt{\frac{M\Omega^2}{2\pi k_B T}} \exp \left[-\frac{M\Omega^2(R - \bar{R})^2}{2k_B T} \right]$$

$$\hat{H}_{\text{elec}} = -\frac{1}{2} \sum_{I=1}^N \sum_{i=1}^n \frac{Z_I}{r_{Ii}}$$

$$E = \langle \Psi | \hat{H} | \Psi \rangle$$

$$\text{KIE} \approx \frac{|S_{\text{H}}|^2}{|S_{\text{D}}|^2} \exp \left\{ -\frac{2k_B T}{M\Omega^2} (\alpha_{\text{D}}^2 - \alpha_{\text{H}}^2) \right\}$$

$$\hat{H}_{\text{nuc}} = -\frac{1}{2} \sum_{I=1}^N \frac{1}{M_I} \nabla_I^2 + \sum_{I < J}^N \frac{Z_I Z_J}{r_{IJ}}$$

$$k^{\text{EPT}} = \sum_{\mu} P_{\mu} \sum_{\nu} \frac{|V^{\text{el}} S_{\mu\nu}|^2}{\hbar} \sqrt{\frac{\pi}{k_B T \lambda}} \exp \left[-\frac{(\Delta G_{\mu\nu}^\circ + \lambda)^2}{4\lambda k_B T} \right]$$

$$k = \frac{k_B T}{h} e^{\Delta G^\ddagger / k_B T}$$