2F4Y: Molecular Structure and Energy Levels

Formula Sheet

Topic 1: Quantum Mechanics

Principles

$$\lambda = \frac{h}{P}$$

$$\Delta P \Delta x \geq \frac{h}{4\pi}$$

$$\psi = wavefunction$$

$$|\psi|^2 = probability = \psi * \psi$$

$$\psi * = complex\ congugate\ (same\ as\ \psi\ but\ \boldsymbol{i} \rightarrow -\boldsymbol{i})$$

ψ must be finite, continuous and single valued

Particle in a One Dimensional Box

$$\psi = d_1 coskx + d_2 sinkx$$

$$\psi = \left(\frac{2}{L}\right)^{\frac{1}{2}} sin\left(\frac{n\pi x}{L}\right) \textbf{\textit{For particle in 1D Box square, and integrate between fractional values of L}}$$

Note: $\int sin^2 ax = \frac{x}{2} - \frac{1}{4a} sin2ax$

Therefore as an example probability between a third and two thirds of box =

$$\left(\frac{2}{L}\right)\left[\frac{x}{2} - \frac{L}{4\pi} sin\frac{2\pi x}{L}\right]_{x=\frac{L}{3}}^{x=\frac{2L}{3}}$$

Average Position $\frac{2}{L}\int_0^L x\ .sin^2 \frac{\pi x}{L} dx$

Energy of a level $E = \frac{n^2\pi^2\hbar^2}{2mL^2}$

Polyenes

$E = \frac{(n_2^2 - n_1^2)h^2}{8mL^2}$ Where n_1 = HOMO and n_2 = LUMO

Quantum Tunnelling

Region I : $\psi = Ae^{ikx} + Be^{-ikx}$ $\qquad$ $k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$

Region II : $\psi_{II} = Ce^{k_{II}x} + De^{-k_{II}x}$ $\qquad$ $k_{II} = \left(\frac{2m(V-E)}{\hbar^2}\right)^{1/2}$

Region III : $\psi = Ee^{ikx}$

A + B = C + D at x = 0 and x = L (Boundary conditions)

$Ce^{k_{II}L} + De^{-k_{II}L} = Ee^{ikL}$

$T = \frac{A^2}{E^2} = \left\{1 + \frac{(e^{k_{II}L} - e^{-k_{II}L})^2}{16\left(\frac{E}{V}\right)\left[1-\frac{E}{V}\right]}\right\}^{-1}$ where $k_{II} = \left(\frac{2m(V-E)}{\hbar^2}\right)^{1/2}$

Scanning Tunnelling Microscopy

$$T = 16\left(\frac{E}{V}\right)\left[1 - \left(\frac{E}{V}\right)\right]e^{-2k_{II}L}$$

Energy Levels of the Simple Harmonic Operator

$E_0 = \frac{\hbar\omega}{2}$ $\qquad$ $E_v = \left(v + \frac{1}{2}\right)\hbar\omega_0$

Variance

$(\Delta x)^2 = \sigma^2 = \langle x^2\rangle - \langle x\rangle^2$ $\qquad$ $\langle x^2\rangle = \frac{L^3}{3} - \frac{L^2}{2\pi^3}$

Therefore

$$\Delta x = L\left(\frac{1}{12} - \frac{1}{2\pi^3}\right)^{1/2}$$

$$\Delta x \Delta p_x = \hbar\left[\frac{n^2\pi^2}{12} - \frac{1}{2}\right]^{1/2}$$
