

1 Atomic Structure

1.1 Energy

$$u_v dv = \frac{8\pi v^2}{c^3} \cdot \frac{hv}{e^{\frac{hv}{k_b T}} - 1} \quad (1)$$

$$E = hv \quad (2)$$

1.2 Photoelectric Effect

$$\frac{1}{2}m_e v_k^2 = E_k = hv - W \quad (3)$$

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad (4)$$

$$R_H = 1.097373 \times 10^7 m^{-1} \quad (5)$$

$$n_1 = 1 \Rightarrow \textit{Lyman} \quad (6)$$

$$n_1 = 2 \Rightarrow \textit{Balmer} \quad (7)$$

$$n_1 = 3 \Rightarrow \textit{Paschen} \quad (8)$$

$$n_1 = 4 \Rightarrow \textit{Brackett} \quad (9)$$

$$n_1 = 5 \Rightarrow \textit{Pfund} \quad (10)$$

$$n_2 > n_1 \quad (11)$$

1.3 De Broglie Relationship

$$E^2 = p^2 c^2 + m^2 c^4 \quad (12)$$

$$\text{for zero rest mass: } E^2 = p^2 c^2 \rightarrow E = pc \quad (13)$$

$$hv = h \frac{c}{\lambda} = pc \quad (14)$$

$$\therefore p = \frac{h}{\lambda} \quad (15)$$

1.4 Electron diffraction

$$E_K = eV - \frac{p^2}{2m} \quad (16)$$

$$p = \sqrt{2meV} \quad (17)$$

$$\lambda = \frac{h}{\sqrt{2meV}} \quad (18)$$

$$\lambda = 2d \sin(\theta) \quad (19)$$

$$\sin^2(\theta) = \frac{C}{V}, \text{ Where } C = \frac{h^2}{8med^2} \quad (20)$$

1.5 Bohr Model

$$F_{centripetal} = F_{electric} \quad (21)$$

$$m \frac{v^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \quad (22)$$

$$\therefore v^2 = \frac{e^2}{4\pi\epsilon_0 mr} \quad (23)$$

$$I_{orbit} = n\lambda = 2\pi r \text{ Where } n \text{ is the quantisation condition} \quad (24)$$

$$\therefore v = \frac{hn}{2\pi mr} \quad (25)$$

$$L = mvr = n \frac{h}{2\pi} = n\hbar \quad (26)$$

$$\text{As such, allowed radii are described by the expression:} \quad (27)$$

$$r_n = \frac{h^2 \epsilon_0 n^2}{\pi m e^2} = a_{Bohr} n^2 \quad (28)$$

$$r_1 = a_{Bohr} = \frac{h^2 \epsilon_0}{\pi m e^2} = 5.3 \times 10^{-11} m \quad (29)$$

$$E_k = \frac{1}{2} m v^2 = \frac{e^2}{8\pi\epsilon_0 r} \quad (30)$$

$$E_T = E_k + E_c = \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r^2} = -\frac{e^2}{8\pi\epsilon_0 r} \quad (31)$$

$$\text{Substituting in } r_n \text{ gives:} \quad (32)$$

$$E_T = - \left(\frac{m e^4}{8 \epsilon_0^2 h^2} \right) \cdot \frac{1}{n^2} = \frac{-13.6 eV}{n^2}, \quad 1 \text{ eV} \approx 1.602 \times 10^{-19} J \quad (33)$$

$$\Delta E = E_i - E_f = \frac{m e^4}{8 \epsilon_0^2 h^2} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \quad (34)$$

$$\text{since: } E = h\nu = h \frac{c}{\lambda} \quad (35)$$

$$\frac{1}{\lambda} = \frac{m e^4}{8 \epsilon_0^2 h^3} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \quad (36)$$

1.6 Waves

$$\Psi = Ae^{i(kx - \omega t)} \quad (37)$$

$$k = 2\pi/\lambda \quad (38)$$

$$\omega = 2\pi v \quad (39)$$

$$c = v\lambda = \frac{\omega}{2\pi} \cdot \lambda = \frac{\omega}{\lambda} \quad (40)$$

$$P(x) \propto |\Psi|^2 dx \quad (41)$$

$$\frac{\partial \Psi}{\partial x} = ikAe^{i(kx - \omega t)} = ik\Psi \quad (42)$$

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx - \omega t)} = i\omega\Psi \quad (43)$$

$$\text{De Broglie: } p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k \quad (44)$$

$$\text{Einstein: } E = hv = h\frac{\omega}{2\pi} = \hbar\omega \quad (45)$$

$$\frac{\partial}{\partial x}\Psi = i\frac{p}{\hbar}\Psi \Rightarrow p\Psi = \{-i\hbar\frac{\partial}{\partial x}\}\Psi \quad (46)$$

$$\frac{\partial}{\partial t}\Psi = -i\frac{E}{\hbar}\Psi \Rightarrow E\Psi = \{i\hbar\frac{\partial}{\partial t}\}\Psi \quad (47)$$

$$\Delta t = \frac{1}{\Delta f} = \frac{h}{\Delta E} \Rightarrow \Delta E \cdot \Delta t \geq h \quad (48)$$

$$\Delta x = \Delta\lambda_{dB} = \frac{h}{\Delta p} \Rightarrow \Delta x \cdot \Delta p \geq h \quad (49)$$

Heisenber's Uncertainty Principle:

It is impossible to specify simultaneously, with precision, both the momentum and the position of a particle.

1.7 Shrodinger's Equation Derivation

$$E = E_k + E_p = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V \quad (50)$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x, t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x, t) + V\Psi(x, t) \quad (51)$$

1.8 Time independent Shrodinger's Equation

$$\Psi(x, t) = \phi(t)\psi(x) \quad (52)$$

$$i\hbar \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = -\frac{\hbar^2}{2m\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V \quad (53)$$

$$\therefore i \frac{A}{\hbar} \phi = \frac{\partial \phi(t)}{\partial t} \quad (54)$$

$$\phi(t) = C e^{-i(\frac{A}{\hbar})t} \Rightarrow \frac{d\phi(t)}{dt} = -i(\frac{A}{\hbar}) C e^{-i(\frac{A}{\hbar})t} \quad (55)$$

$$\text{By unit analysis: } A = E \quad (56)$$

$$\therefore E\psi = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi \quad (57)$$

1.9 Electron in a box

$$V(0) = V(L) = \inf \quad (58)$$

$$V(x) = 0 \quad \forall x \mid 0 < x < L \quad (59)$$

$$\therefore -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E\psi \quad (60)$$

$$\text{General Solution: } \psi = A \sin(kx) + B \cos(kx) \quad (61)$$

$$\frac{d^2 \psi}{dx^2} = -k^2 (A \sin(kx) + B \cos(kx)) = -k^2 \psi \quad (62)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = \left(-\frac{\hbar^2}{2m} \right) \cdot (-k^2 \psi) = E\psi \quad (63)$$

$$E = \frac{\hbar^2 k^2}{2m} \quad (64)$$

$$\text{Applying boundary conditions:} \quad (65)$$

$$\psi(0) = 0 \Rightarrow B = 0 \quad (66)$$

$$\psi(L) = 0 \Rightarrow A = 0 \text{ or } \sin(kL) = 0 \quad (67)$$

$$\therefore kL = n\pi, \quad n = 1, 2, 3, \dots \quad (68)$$

$$\psi_n = A \sin\left(\frac{n\pi x}{L}\right) \quad (69)$$

$$E_n = \frac{\hbar^2}{8mL^2} \cdot n^2 \quad (70)$$

$$1 = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx \Rightarrow A = \sqrt{\frac{2}{L}} \quad (71)$$

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (72)$$

$$P_n(x) = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) dx \quad (73)$$

1.10 3D

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) \psi + V\psi = E\psi \quad (74)$$

$$\nabla = \left(\frac{d}{dx} + \frac{d}{dy} + \frac{d}{dz} \right) \quad (75)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi \quad (76)$$

There are 3 spacial degrees of freedom and 1 spin degree of freedom, therefore there are 4 quantum numbers

n = Principle quantum numbers, $\{n \mid n \in \mathbb{N}\}$

ℓ = Orbital quantum number $\{\ell \mid 0 \leq \ell \leq n-1, \ell \in \mathbb{W}\}$

m_ℓ = Magnetic quantum number $\{m_\ell \mid -\ell \leq m_\ell \leq \ell, m_\ell \in \mathbb{Z}\}$

m_s = Spin quantum number $\{m_s \mid m_s \in \{\frac{1}{2}, -\frac{1}{2}\}\}$

2 Bonding and Crystalline Structure