

Inorganic Chemistry

Q.S.-Part-I, Group-B

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Schrodinger's Wave equation

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Lecture Notes Series:-

Based on the idea of de-Broglie (dual nature of matter), Schrodinger in 1926 derived the following wave equation for a moving particles.

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m (E - V)}{\hbar^2} \psi = 0$$

where 'm' is the mass of the Electron 'E' and 'V' are the total Energy and the Potential energy of the electron 'h' is the Planck constant and ψ is the wave function.

The above equation is known as Schrodinger wave equation

Derivation:

The wave equation of stationary wave associated with the particles in terms of Cartesian co-ordinates system at any instant is given by

$$\psi = A \sin \frac{2\pi x}{\lambda} \quad \text{--- (1)}$$

Where ψ = Wave function

A = Maximum value of ψ

x = Distance from the nucleus

λ = Wave length

Differentiating equation (1) with respect to x, we get

$$\frac{d\psi}{dx} = A \cos \frac{2\pi x}{\lambda} \cdot \left(\frac{2\pi}{\lambda} \right)$$

$$\text{or } \frac{d\psi}{dx} = \frac{2\pi A}{l} \cdot \cos \frac{2\pi x}{l} \quad \text{--- (2)}$$

Differentiating again equation (2) and with respect to x , we have.

$$\frac{d^2\psi}{dx^2} = - \frac{2\pi A}{l} \sin \frac{2\pi x}{l} \left(\frac{2\pi}{l} \right)$$

$$\text{or } \frac{d^2\psi}{dx^2} = - \frac{4\pi^2 A}{l^2} \sin \frac{2\pi x}{l} \quad \text{--- (3)}$$

From eq (1) and (3) we get

$$\frac{d^2\psi}{dx^2} = - \frac{d^2\psi}{dx^2}$$

$$\text{or, } \frac{1}{l^2} = - \frac{d^2\psi}{dx^2} \times \frac{1}{4\pi^2 A} \quad \text{--- (4)}$$

combining this eqs with de-Broglie eq 1 =

$$\frac{h}{Mv} \propto \frac{1}{l^2} = \frac{M^2 v^2}{h^2} \quad (\text{M = Mass of electron})$$

v = velocity of electron) we get

$$\frac{M^2 v^2}{h^2} = - \frac{d^2\psi}{dx^2} \times \frac{1}{4\pi^2 A}$$

$$\text{or, } M^2 v^2 = - \frac{h^2}{4\pi^2 A} \cdot \frac{d^2\psi}{dx^2}$$

$$\text{or, } \frac{1}{2} M v^2 (K.E.) = - \frac{h^2}{8\pi^2 A} \cdot \frac{d^2\psi}{dx^2} \quad \text{--- (5)}$$

Now the total Energy (E) of the particle is the sum of Kinetic Energy and Potential Energy i.e

$$E = K.E + P.E$$

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$$\therefore E = - \frac{\hbar^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + V$$

$$\left[\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{\hbar^2} (E - V) \psi = 0 \right] \quad (1)$$

This is Schrodinger wave equation in one dimension X, In three dimensions x, y, z the equation written as

$$\left[\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{\hbar^2} (E - V) \psi = 0 \right]$$