

Quantum Chemistry

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Explain the shape of electron movement.

$$\nabla^2 \Psi = \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} \quad (1)$$

$$\nabla^2 \phi + \frac{2m}{\hbar^2} (E - V) \phi = 0 \quad (2)$$

$$\hat{H} \Psi = i \hbar \frac{\partial \Psi}{\partial t} \quad (3)$$

$$\frac{\partial^2 \phi_{tr}}{\partial X^2} + \frac{\partial^2 \phi_{tr}}{\partial Y^2} + \frac{\partial^2 \phi_{tr}}{\partial Z^2} + \frac{2M}{\hbar^2} E_{tr} \phi_{tr} = 0 \quad (4)$$

$$\phi_T = \phi_{tr}(X, Y, Z) \phi(x, y, z) \quad (5)$$

$$\nabla^2 \phi + \frac{2\mu}{\hbar^2} (E + \frac{Ze^2}{r}) \phi = 0 \quad (6)$$

$$\phi = \phi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad (7)$$

$$\frac{d^2 \Phi}{d\phi^2} + m^2 \Phi = 0, m = 0, \pm 1, \pm 2 \dots \quad (8)$$

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} \exp(im\phi) \quad (9)$$

$$\Theta_{lm}(\theta) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{(2l+1)(l-|m|)!}{2(l+|m|)!}} P_l^{|m|}(\cos\theta) \quad (10)$$

$$R_{nl}(r) = -\sqrt{\frac{2Z}{na_0} \frac{(n-l-1)!}{2n((n+l)!)^3}} \exp(-\rho/2) \rho^l L_{n+l}^{2l+1}(\rho) \quad (11)$$

$$\rho = \frac{2Z}{na_0} r, a_0 = \frac{\hbar^2}{\mu e^2} \quad (12)$$

$$\begin{aligned} n &= 1, 2, 3, 4 \dots \\ l &= 0, 1, 2, 3, \dots, n-1 \\ m &= 0, \pm 1, \pm 2, \dots, \pm l \end{aligned} \quad (13)$$

$$\phi_{1s} = \frac{1}{\sqrt{\phi}} \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}, n=1, l=0, m=0 \quad (14)$$