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[illegible]
Physical Chemistry

Solution of Φ equation —

The Φ equation is

$$\frac{1}{\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} = -m^2$$

or

$$\frac{\partial^2 \Phi}{\partial \phi^2} + m^2 \Phi = 0$$

Φ = function of ϕ
ϕ = angle

It is the second order differential equation which solution is —

$$\Phi = A e^{\pm im\phi}$$

Since Φ must be normalised, where A = const.

$$\int_0^{2\pi} \Phi \Phi^* \, d\phi = 1$$

or, $$\int_0^{2\pi} A e^{+im\phi} \cdot A e^{-im\phi} \cdot d\phi = 1$$

or, $$A^2 \int_0^{2\pi} d\phi = 1$$

or, $$A^2 [\phi]_0^{2\pi} = 1$$

or, $$A^2 \times 2\pi = 1$$

or $$A = \sqrt{\frac{1}{2\pi}} = \frac{1}{\sqrt{2\pi}}$$

$$\therefore \Phi = A e^{\pm im\phi}$$

$$= \frac{1}{\sqrt{2\pi}} e^{\pm im\phi}$$

In order that Φ be a single valued function position it should have same value at ϕ = [illegible] and $\phi = 2\pi$

ie, $$\Phi(\phi) = \Phi(\phi + 2\pi)$$

$$\therefore \Phi = A e^{\pm im\phi} = A \cdot e^{\pm im(\phi + 2\pi)}$$

or, $Ae^{\pm im\phi} = Ae^{\pm im\phi} \cdot e^{\pm 2\pi im}$

or, $e^{\pm 2\pi im} = 1$

or, $\cos 2\pi m \pm i \sin 2\pi m = 1$

which is the only if m is an integer

i.e., $m = 0, \pm 1, \pm 2, \pm 3 \ldots\ldots$

m is known as magnetic quantum number. m gives the energy of a H-atom in a mag. field.

for $m = 0$,

$$\phi = \frac{1}{\sqrt{2\pi}} \cdot e^{\pm im\phi}$$

$$= \frac{1}{\sqrt{2\pi}}$$

for $m = \pm 1, \pm 2, \pm 3 \ldots\ldots$

$$\phi = \frac{1}{\sqrt{2\pi}} e^{\pm im\phi}$$

$$= \frac{1}{\sqrt{2\pi}} \left(\cos m\phi + i \sin m\phi \right)$$

Solution of Θ equation :→

The Θ equation is —

$$\frac{1}{\sin\theta} \cdot \frac{d}{d\theta}\left(\sin\theta \cdot \frac{d\Theta}{d\theta}\right) + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)\Theta = 0$$

Where Θ = function and θ = angle,

the equation has the soln

$$\Theta = B\, P_l^m \cos\theta$$

Where

B = normalising const.

and $P_l^m \cos\theta$ is the associated ~~Leg~~ Legendre Polynomial of degree l and order m.

$$B = \sqrt{\left[\frac{(2l+1)}{2} \cdot \frac{(l-m)!}{(l+m)!}\right]}.$$

and $$P_l^m \cos\theta = (1-\cos^2\theta)^{m/2} \cdot \frac{d^m}{dx^m} P_l(\cos\theta)$$

where $P_l \cos\theta$ is ~~the~~ Legendre Polynomial ~~equation~~ of degree l.

$$P_l(\cos\theta) = 2^{1/l} \cdot (l!) \frac{d^l}{(d\cos\theta)^l} (\cos^2\theta - 1)^l$$

where l is an ~~integer~~ integer

$$l = |m|, |m|+1, |m|+2, \ldots$$

where $|m|$ = absolute value of m

and $\lambda = l(l+1)$

l is known as azimuthal quantum no. The angular momentum associated with a particular value of l is given by $\rightarrow$ $\sqrt{l(l+1)} \cdot h/2\pi$.

Solution of R - equation :→

The equation for Radial wave function is —

$$\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) + \left[\frac{2\mu}{\hbar^2}(E - V) - \frac{\lambda}{r^2}\right] R = 0$$

where $V = \frac{-Ze^2}{r}$ = pot. energy.

$\lambda = l(l+1)$

The solution is —

$$R = C e^{-\rho/2} \cdot \rho^l \cdot L_{n+l}^{2l+1}(\rho)$$

where C = normalising const.

$\rho = 2Zr/na_0$

where a_0 = Bhor