

$$U = \frac{1}{2} \mu v^2 = \frac{1}{2} \mu r^2 \left(\frac{v}{r} \right)^2 = \frac{1}{2} I \omega^2 = \frac{(I\omega)^2}{2I} = \frac{L^2}{2I} \quad (1)$$

where I is the moment of inertia, $I = \mu r^2$, ω is the angular velocity, $\omega = v/r$, and L is the angular momentum, $L = I\omega$.

$$\hat{H} = \frac{1}{2I} \hat{L}^2 \quad (2)$$

$$\hat{H} = \frac{1}{2I} (-\hbar^2) \left\{ \frac{1}{\sin\theta} \left[\frac{\partial}{\partial\theta} (\sin\theta) \frac{\partial}{\partial\theta} \right] + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right\} \quad (3)$$

$$\hat{H} \Psi = -\frac{\hbar^2}{2I} \left\{ \frac{1}{\sin\theta} \left[\frac{\partial}{\partial\theta} (\sin\theta) \frac{\partial}{\partial\theta} \right] + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right\} \Psi = \varepsilon \Psi \quad (4)$$

The solutions to equation (4), Ψ_{Jm} , depend on both θ and ϕ , and can be written as a product of two functions, one in θ and one in ϕ .

$$\Psi_{Jm} = \Theta_{Jm} \Phi_m \quad J = 0, 1, 2, \dots \quad m = 0, \pm 1, \pm 2, \pm 3, \dots, \pm J \quad (5)$$

$$\Phi_m = \sqrt{\frac{1}{2\pi}} e^{im\phi} \quad (6)$$

Θ_{Jm} = normalized associated Legendre polynomials (see Appendix, Table A.4)

$$\Theta_{Jm} = f(J, m, \theta) \quad J = 0, 1, 2, \dots \quad m = 0, \pm 1, \pm 2, \pm 3, \dots, \pm J \quad (7)$$

The first two normalized associated Legendre polynomials are:

$$\Theta_{00} = \frac{\sqrt{2}}{2} \quad \Theta_{10} = \frac{\sqrt{6}}{2} \cos(\theta)$$

The rotational energies, ε_J , are given by:

$$\varepsilon_J = \frac{\hbar^2}{2I} J(J+1) \quad I = \mu r^2 \quad (8)$$

Solve the following

- For Ψ_{00} , show that equation (4) yields the value of the energy as given by equation (8).
- For Ψ_{10} , show that equation (4) yields the value of the energy as given by equation (8).
- How many nodes are there in Ψ_{00} ? Ψ_{10} ? Comment on the relationship between the number of nodes in the rotational wavefunction and the corresponding rotational energy.
- What is the degeneracy of the $J = 19$ level for a rigid rotor?

Answers Chemactivity 6

Richard Samuel Moog



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