The general schrödinger equation in spherical polar co-ordinates is given by

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)$$

$$+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \quad (3)$$

As r is constant (=1), hence the factor $\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)=0$, and since there is no force acting on the rotator, $V=0$. Therefore, eqn. (3) becomes,

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2I}{\hbar^2}E\psi=0 \quad (4)$$

This eqn. consists of two variable θ and ϕ which represent the precessional motion of the rotators free axis and the rotation of the system respectively.

Eigen values:

The corresponding eigen value of ψ_{lm} is given by

$$\beta = l(l+1)$$

or, $$\frac{2IE_l}{\hbar^2}=l(l+1)$$

$$\therefore \quad E_l = \frac{\hbar^2}{2I}\, l(l+1), \quad \text{where } l = 0, 1, 2, 3 \quad (5)$$

Thus we conclude that the Schrödinger equation for the rigid rotator can have physically acceptable solutions only for certain discrete values of energy called energy eigen values represented by eqn. (5).

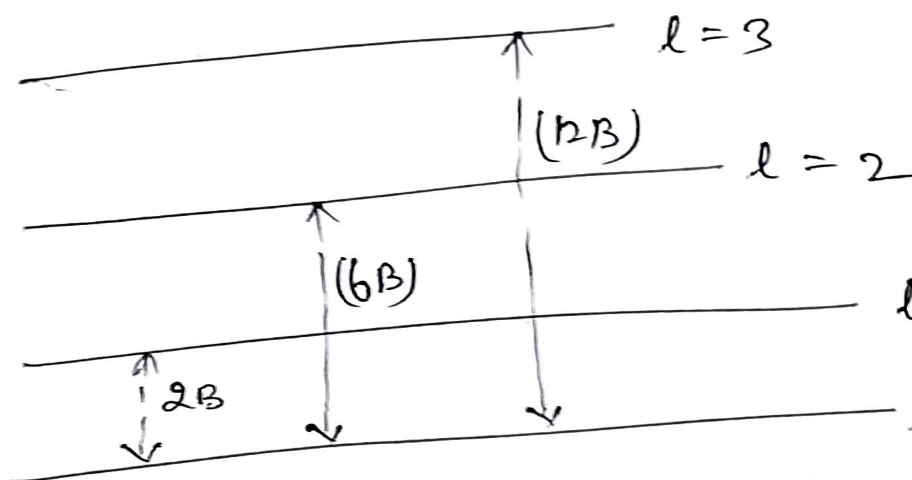

fig-(2) Energy level diagram of a rigid rotator.

When, $l = 0$, $E_0 = 0$

$l = 1$, $E_1 = \frac{\hbar^2}{2I} \cdot 2 = 2B$ (say)

$l = 2$, $E_2 = \frac{\hbar^2}{2I} \cdot 6 = 6B$ (say)

$l = 3$, $E_3 = \frac{\hbar^2}{2I} \cdot 12 = 12B$ (say)

The energy level diagram is shown in fig. (2). It is observed from the figure that the energy levels have a characteristic ratios exhibited by the diatomic molecules due to rotational motion.

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