

$$\therefore I = m_1 \left(\frac{m_2 r}{m_1 + m_2} \right)^2 + m_2 \left(\frac{m_1 r}{m_1 + m_2} \right)^2$$

$$\text{or, } I = \left(\frac{m_1 m_2}{m_1 + m_2} \right) r^2$$

$$= \mu r^2 \quad \text{--- (4)}$$

where, $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is called the reduced mass of the system.

The K.E. of rotation is

$$E_r = \frac{1}{2} I \omega^2 \quad \text{--- (5)}$$

where ω is the angular velocity of the system. Since the molecule is rigid, the p.e. is zero. i.e.; $V = 0$. The quantised energy levels of rotation are obtained by solving the Schrodinger equation

$$\nabla^2 \psi + \frac{8\pi^2 \mu E}{h^2} \cdot \psi = 0 \quad \text{--- (6)}$$

The appropriate and acceptable solution of this equation yields that

$$E = \frac{h^2}{8\pi^2 I} \cdot J(J+1) \quad \text{--- (7)}$$

where J is the rotational quantum number having integral values 0, 1, 2, 3, ...

For a given species of molecule, $\frac{h^2}{8\pi^2 I}$ is a constant and is called the Rotational constant.

Let us put $\frac{h}{8\pi^2 I} = B$.

$$\therefore E = B h \cdot j(j+1) \text{ ————— (8)}$$

The difference in energy between two rotational levels j and j' .

$$\Delta E = B h j(j+1) - B h j'(j'+1) \text{ ————— (9)}$$

There are two restrictions in such rotational transitions .

1) According to electrodynamic considerations, the absorption or emission of a radiation in rotational level would occur only if a charge is dipole moment of the molecule is associated with it. This means that the molecule must be polar, in order to produce a rotational spectrum. Homopolar molecules like H_2 , N_2 , Cl_2 --- etc have no rotational band. This restriction also applies to vibrational quantum level changes.

2) The transition in rotational energy is limited to adjacent levels, i.e;

$$\Delta j = \pm 1 .$$

Since, $j - j' = 1$ eqn (9) takes the form

$$\Delta E = B h j(j+1) - B h (j-1)j = 2 B h j \text{ ————— (10)}$$