Give an account of Rotational spectra of a diatomic molecule.

Let us consider a rotation in diatomic molecule regarded as a rigid rotator. The two atoms A and B are at a distance r as shown in fig-(1).

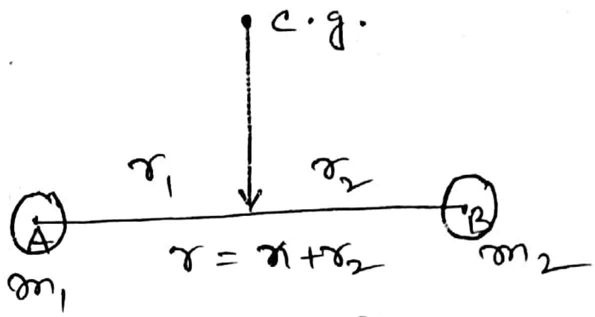

Fig-(1)

If r_1 and r_2 be the distance of the two atoms from the centre of gravity (c.g) of the system, then the moment of inertia of the system is given by

$$I = m_1 r_1^2 + m_2 r_2^2 \qquad \text{——— (1)}$$

We know that about the c.g.,

$$m_1 r_1 = m_2 r_2$$

$$m_1 r_1 = m_2 (r - r_1) \qquad [\because r = r_1 + r_2]$$

$$\therefore r_1 = \frac{m_2 r}{m_1 + m_2} \qquad \text{——— (2)}$$

Similarly, $$r_2 = \frac{m_1 r}{m_1 + m_2} \qquad \text{——— (3)}$$

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

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

$$= \mu r^2 \quad \text{——— (4)}$$

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 schroodinger 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 molecules, $\frac{h}{8\pi^2 I}$ is a constant and is called the Rotational constant.