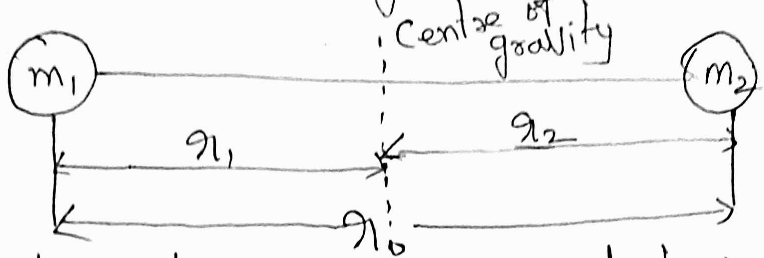
Unit - IV

(1)

1. Derive an expression for the rotational energy of a molecule taking it as a rigid rotator. Draw the rotational energy level diagram for such a molecule.

On the basis of wave mechanics, it can be seen that a diatomic molecule is considered as a rigid rotator.



* Centre of gravity of a diatomic molecule is the point which satisfies the following:

$$m_1 r_1 = m_2 r_2 \quad \text{------} \rightarrow (1)$$

The moment of inertia of the diatomic molecule is

$$I = m_1 r_1^2 + m_2 r_2^2 \quad \text{------} \rightarrow (1)\text{-}A$$

$$= m_2 r_2 r_1 + m_1 r_1 \cdot r_2$$

$$= r_1 \cdot r_2 (m_2 + m_1) \longrightarrow (2)$$

but $r_0 = r_1 + r_2$

$$\boxed{\therefore r_0 - r_1 = r_2} \quad \text{------} \rightarrow (3)$$

$$\therefore r_1 = \left(\frac{m_2}{m_1 + m_2}\right) r_0$$

$$r_2 = \left(\frac{m_1}{m_1 + m_2}\right) r_0$$

… of r_1 & r_2 in (1) A (2)

$$I = \mu r_0^2 \left\{ \text{where } \mu = \frac{m_1 . m_2}{m_1 + m_2} \right\} \quad \text{--→ (4)}$$

∴ Angular momentum of a rotating molecule is given by

$$L = I\omega \text{ ------→ (5)}$$

ω → angular velocity

∴ The quantized angular momentum is

$$L = \sqrt{J(J+1)}\,\frac{h}{2\pi} \text{ ------→ (6)}$$

∴ Energy of rotating molecule is given by

$$E = \frac{1}{2} I\omega^2$$

$$= \frac{1}{2\times I}\, I^2\omega^2 = \frac{L^2}{2I} \text{ ------→ (7)}$$

∴ From eqn (6)

$$L^2 = J(J+1)\times\frac{h^2}{4\pi^2} \text{ ------→ (8)}$$

Subsitute eqn (8) in (7)

$$\therefore E = J(J+1)\times\frac{h^2}{4\pi^2}\times\frac{1}{2I}$$

$$\boxed{E = \frac{h^2}{8\pi^2 I}\, J(J+1)} \text{ ------→ (9)}$$

<u>Rotational energy level diagram</u>

where $J = 0, 1, 2, 3 \ldots$

J → Rotational quantum no

- 3 ——— $12h^2/8\pi^2 I$
- 2 ——— $6h^2/8\pi^2 I$
- 1 ——— $2h^2/8\pi^2 I$
- 0 ——— 0