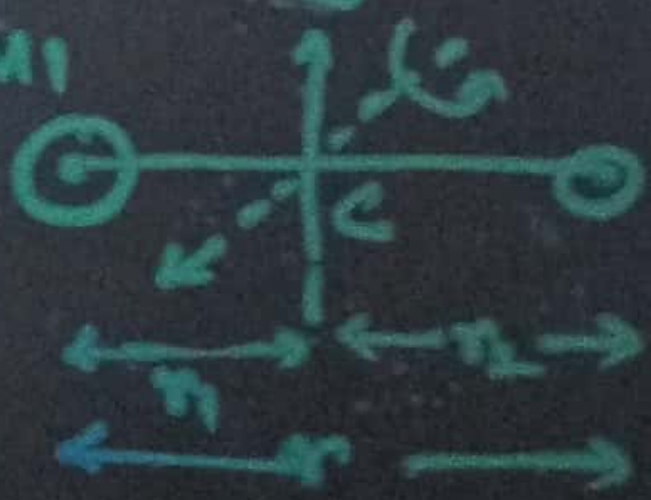
Quantisation of Rotational Energies, Pure Rot. Spectra

→ Hetronuclear Molecules like HCl, HF, CO etc

→ Exhibit Absorption & spectral lines in FIR region

→ freq interval between two successive lines are same (2B)

→ Diatomic molecule may rotate about its axis joining two nuclei



$m_1 r_1 = m_2 r_2$

&

$r_1 + r_2 = r$

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Such that:

$$m_1 r_1 = m_2 r_2$$

and $$r_1 + r_2 = r$$

then; $r_1 = \frac{m_2 r}{m_1 + m_2}$ & $r_2 = \frac{m_1 r}{m_1 + m_2}$

Hence;

M.O.I about an axis passing through 'c' and ⊥r to axis joining atoms —

$$I = m_1 r_1^2 + m_2 r_2^2$$

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

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

$$\boxed{I = \mu r^2} \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

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⇒ Molecule (Diatomic)

↳ can be considered as a particle of mass μ rotating about the axis with an ang. velocity 'ω' and ang. momentum P:

then, $P = I\omega$

& KE of the molecule

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

∵ 'r' distⁿ. betⁿ. atoms in the molecule does not change during rotation

PE = remains same (but) = 0

Tot Energy $E = \frac{1}{2} I \omega^2 = (KE)$

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Thus,

$$E = \frac{1}{2} I \left(\frac{P}{I}\right)^2$$

$$E = \frac{P^2}{2I}$$

Accord. to Q.M; P is quantized

$$P = \sqrt{j(j+1)}\,\frac{h}{4\pi}$$

where, $j = 0, 1, 2, 3 \ldots$ rot. Q. No.

$$E_j = \frac{j(j+1)\,h^2}{8\pi^2 I}$$

or, $$\boxed{E_j = j(j+1)\,B}$$

$B = \frac{h^2}{8\pi^2 I}$ → Rot. const of the Molecule.

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B (Rotational const.)

→ Diff for diff molecules
→ Characteristic property of Molecule
→ Unit of Energy (Joule)
→ Give info abt MoI of molecule.

Thus: Rotational Energy states of a molecule is quantized i.e. not continous but discrete.

if $j = 0$; $E_0 = 0$
$j = 1$; $E_1 = 2B$
$j = 2$; $E_2 = 6B$
$j = 3$; $E_3 = 12B$

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→ Energy states are not equi-spaced

→ Energy Interval between two consq. states increases

→ Lowest Energy $E_0 = 0$

→ Min. energy released;

$$E_1 - E_0 = -2B$$

→ freq corresponding to $E_1 \to E_0$ transition =

$$\nu = \frac{E_1 - 0}{h} = +\frac{2B}{h}$$

→ freq corresponding to this min diff in energy

$$\boxed{\nu = \frac{2B}{h}} \quad \text{or} \quad \boxed{\lambda = \frac{hc}{2B}}$$

thus

→ for HCL; $2B \simeq 0.0026$ eV

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