P-1

21 — 4th Week • 021-345 — JANUARY — Tuesday

Sem-6 (H) DRG

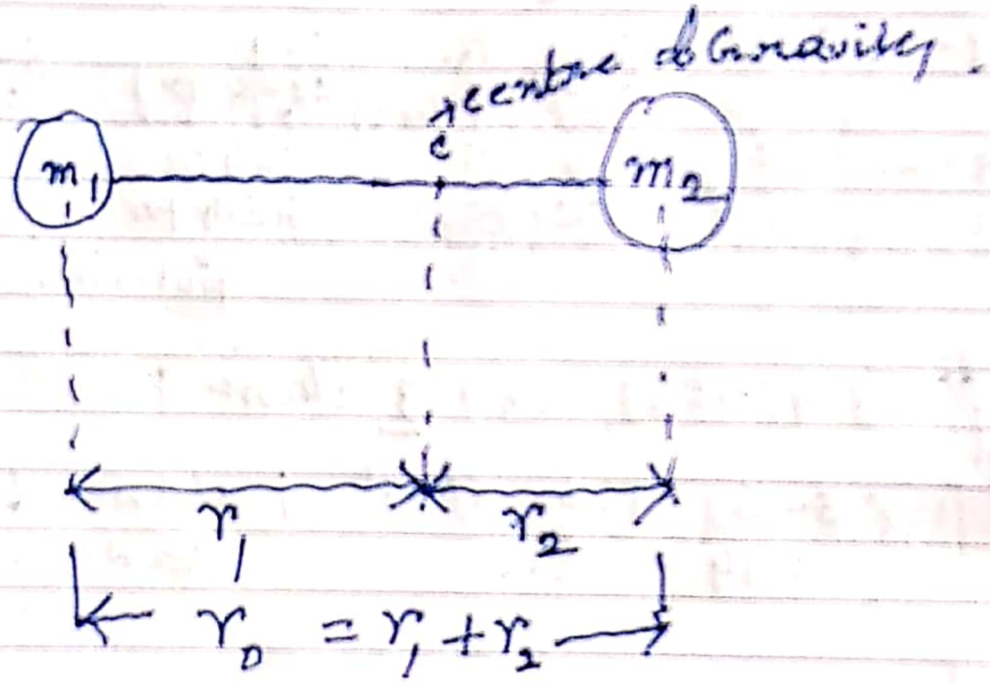
CC-14

(class-2)

Topic

# Rotional Energy

Centre of gravity of a diatomic molecule is the point whic satisfies the following condition.




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

The moment of inertia

(due to end over end rotation in the plane or perpendicular to the plane of the paper.)

NOTES

of the diatomic molecule is given by $I = m_1 r_1^2 + m_2 r_2^2$ ...... (2)

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

$$= r_1 r_2 (m_1 + m_2) \quad \text{......} (3)$$

But $r_1 + r_2 = r_0$ ...... (4)

From eqn (1) $m_1 r_1 = m_2 (r_0 - r_1)$

$$\therefore m_1 r_1 + m_2 r_1 = m_2 r_0$$

$$\therefore r_1 = \frac{m_2 r_0}{m_1 + m_2} \quad \text{......} (5)$$

Similarly, $r_2 = \frac{m_1 r_0}{m_1 + m_2}$ ...... (6)

Putting the value of $r_1$ and $r_2$ in eqn (3), we get $I = \frac{m_1 m_2 r_0^2}{(m_1 + m_2)^2} (m_1 + m_2)$

$$= \frac{m_1 m_2}{m_1 + m_2} \cdot r_0^2$$



$$= \mu \cdot r_0^2 \quad \text{......} (7)$$

where, $\mu$ = reduced mass = $\frac{m_1 m_2}{m_1 + m_2}$

9.00

Now Angular momentum of a

10.00

rotating molecule is

11.00

$$L = I \cdot \omega \quad \text{-----} \quad (8)$$

12.00

where $\omega$ = Angular Velocity

1.00

But angular momentum is quantised

2.00

$$L = \sqrt{J(J+1)} \cdot \frac{h}{2\pi} \quad \text{---} \quad (9)$$

3.00

4.00 Where J = 0, 1, 2, 3 --- called rotational

5.00 quantum number.

6.00

Energy of a diatomic molecule

is given by

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

NOTES

∴ The quantized value of the rotational energy

$$E_r = \frac{1}{2} I \cdot \omega^2 = \frac{(I\omega)^2}{2I} \quad \ldots (10)$$

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

$$= \frac{h^2}{8\pi^2 I} \cdot J(J+1) \quad \ldots (11)$$

∴ Rotational Energy $= \frac{h^2}{8\pi^2 I} J(J+1)$ ...(11)

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

Agen we know,

$E = h\nu = \frac{hc}{\lambda}$ [∵ $c = \nu\lambda$]

c = velocity of light
ν = Frequency
λ = Wave length

$\therefore \frac{1}{\lambda} = \bar{\nu} = \frac{E}{hc}$

$\frac{1}{\lambda}$ = wave no.

$$\therefore \frac{1}{\lambda} = \bar{\nu} = \frac{E}{hc} = \frac{h}{8\pi^2 I c} J(J+1) \quad \ldots (12)$$

9.00 $\therefore$ Wave No. $= \frac{1}{\lambda} = \bar{\nu} = \frac{h}{8\pi^2 Ic} J(J+1)$ ...(12)

10.00 $$\bar{\nu} = B\,J(J+1)\ \text{cm}^{-1} \quad (13)$$

11.00 where $B = \frac{h}{8\pi^2 I \cdot c}$ is called

12.00 rotational constant.

1.00

2.00 Selection rule — only those

3.00 rotational transitions are

4.00 allowed for which $\Delta J = \pm 1$

5.00

$\Delta\bar{\nu}_{J\,0\to1} = B\cdot1(1+1) - B\cdot0(0+1)$

6.00

$= 2B$ [From eqn (13)] .....(14)



similary $\Delta\bar{\nu}_{J=1\to2} = B\cdot2(2+1) - B\cdot1\cdot(1+1)$

$= 6B - 2B = 4B$ ...(15)

$\Delta\bar{\nu}_{J=2\to3} = B\cdot3\cdot(3+1) - B\cdot2\cdot(2+1) = 6B$ -(16)

NOTES

wave no.s of the lines would be
2B, 4B, 6B and so on.

Thus various lines in the rotational spectra will be equally spaced.
In the rotational spectroscopy two succesive lines have a constant difference of wave number which is equal to 2B.

The essential condition for a molecule to exhibit rotational spectrum is that it must have a permanent dipole moment.
The molecules with permanent dipole moment are known as

NOTES

the microwave active molecules and those with no permanent dipole moment are known as microwave inactive molecules.

Thus homonuclear molecules such as $H_2$, $N_2$, $O_2$ and $Cl_2$ have no permanent dipole moment ~~and hence~~ do not exhibit the rotational spectra. Molecules $CO_2$, $CS_2$, $H-C\equiv C-H$ having centre of symmetry do not possess permanent dipole moment are microwave inactive molecules also.