Micro Wave Spectroscopy:-

* Consider a diatomic molecule m_1 and m_2.
* m_1 & m_2 are mass of the two atom.
* r is the equilibrium bond length.
* Rotating about an axis passing through its Centre of gravity.
* The Centre of gravity is defined by equality of moment. (ie) $m_1 r_1 = m_2 r_2 \rightarrow (1)$
* The moment of Inertia of diatomic molecule

$$I = m_1 r_1^2 + m_2 r_2^2 \rightarrow (2)$$

$$= m_1 r_1 r_1 + m_2 r_2 r_2 \rightarrow (3)$$

equ (1) is subj. in equ (3)

$$= m_2 r_2 r_1 + m_1 r_1 r_2 \rightarrow (4)$$

common term $(r_1 r_2)$

$$I = r_2 r_1 (m_2 + m_1) \rightarrow (5)$$

$$r = r_1 + r_2 \rightarrow (6)$$

(1) → get ⇒ r_1 value

combined

equ (1) and (5) $\cancel{m_1 m}$ $m_1 r_1 = m_2 r_2 = m_2 (r - r_1) \rightarrow (7)$

(7) → get ⇒ r_2 value

From equation (7)

$$\boxed{r_1 = \frac{m_2 r}{m_1 + m_2} \; ; \; r_2 = \frac{m_1 r}{m_1 + m_2}} \rightarrow (8)$$

equation (8) is subj. in equ (2) [r_1 & r_2 Values substitue

equ (2) $I = m_1 r_1^2 + m_2 r_2^2$

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

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

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

$$= \frac{m_1 m_2 r^2 \cancel{(m_2+m_1)}}{(m_1+m_2)^{\cancel{2}}} = \boxed{\frac{m_1 m_2}{m_1+m_2}} r^2 = \mu r^2$$

$$\boxed{I = \mu r^2} \rightarrow (9)$$ μ = reduced mass.

Classically Angular momentum of ~~dia~~ rotating molecule

$$L = I\omega \rightarrow (10)$$

$L \rightarrow$ Angular momentum
$I \rightarrow$ moment of Inertia
$\omega \rightarrow$ angular velocity.

However. $L \rightarrow$ is quantized.

$$L = \sqrt{J(J+1)}\, h/2\pi \qquad J = 0,1,2,3\ldots \rightarrow (11)$$

$\hookrightarrow$ rotational quantum number.

* The Energy of rotating molecule is $\frac{1}{2} I\omega^2$
* Hence quantized Energy of rotating diatomic molecule

$$E_J = \frac{1}{2} I\omega^2 \qquad L = I\omega$$

$$(\times) \text{ by } I/I = (I\omega)^2/2I = L^2/2I. \qquad L^2 = (I\omega)^2$$

so equations (11)

$$E_J = \frac{h^2}{8\pi^2 I} J(J+1) \text{ Joule.} \qquad J = 0,1,2\ldots \rightarrow (12)$$

equations (12) $\div$ by hc.

$$\frac{E_J}{hc} = F(J) = \boxed{\frac{h}{8\pi^2 Ic}} J(J+1)\,\mathrm{cm}^{-1} \qquad J = 0,1,2\ldots \rightarrow (13)$$

$B \rightarrow$ Rotation term.

(i.e) Rotational constant: B

$$B = \frac{h}{8\pi^2 Ic}\ \mathrm{cm}^{-1}$$

$= BJ(J+1) \qquad J = 0, 1, 2, 3 \ldots$

Selection rule:-

* The selection to determine the radiative transitions between the rotational energy levels.

* $\Delta J = \pm 1$

  $+ \rightarrow$ refers to absorption of radiation.

  $- \rightarrow$ refers to emission of radiation.

* Microwave spectra are observed as absorption spectra so that the selection rule is $\boxed{\Delta J = +1}$

* For a transition taking place from J to J+1.

* The rotational frequency is

$$\nu_{(J \to J+1)} = B(J+1)(J+2) - BJ(J+1)$$

$$= B(J^2+3J+2) - B(J^2+J) = 2B(J+1)\,cm^{-1}$$

Thus $\nu_{0 \to 1} = 2B$

$\nu_{1 \to 2} = 4B$

$\nu_{2 \to 3} = 6B$ etc...

We see that the rotational spectrum of rigid diatomic molecule consists of series of lines at

2B, 4B, 6B, 8B etc...

* These lines equally spaced by an amount of 2B called frequency seperation (with draw Diagram)