PROBLEMS :-

1. In CO molecule the wavenumber difference between the successive absorption lines in the pure rotational spectrum is 384 m^{-1}. Calculate moment of Inertia of the molecule and the equilibrium bond length of the molecule.

Given :- Masses of C^{12} atoms = 1.99×10^{-26} Kg

Masses of O^{16} atoms = 2.66×10^{-26} Kg.

W.K.T $\Delta\bar{\nu} = \dfrac{h}{4\pi^2 I C} = 384\ m^{-1}$

$$\therefore \quad I = \frac{h}{4\pi^2 C\,\Delta\bar{\nu}} = \frac{6.654 \times 10^{-34}}{4\pi^2 \times 3 \times 10^8 \times 384}$$

$$I = 1.456 \times 10^{-46}\ \text{Kg m}^2$$

$$\text{Reduced mass } (\mu) = \frac{m_1 m_2}{m_1 + m_2} = \frac{1.99 \times 2.66 \times 10^{-52}}{[1.99 + 2.66] \times 10^{-26}}$$

$$\therefore \quad \mu = 1.138 \times 10^{-26}\ \text{Kg.}$$

$$\text{Bond length } (r) = \sqrt{\frac{I}{\mu}} = \sqrt{\frac{1.456 \times 10^{-46}}{1.138 \times 10^{-26}}} = 0.1131 \times 10^{-9}\ \text{mt}$$

2. The lines in the pure rotational spectrum of HCl are spaced as 20.8×10^2 per metre. Calculate moment of Inertia and the Internuclear distance. Mass of proton = 1.67×10^{-27} Kg, mass of Chlorine = 58.5×10^{-27} Kg.

$$\text{Reduced mass } (\mu) = \frac{m_1 m_2}{m_1 + m_2} = \frac{1.67 \times 10^{-27} \times 58.5 \times 10^{-27}}{(1.67 + 58.5) \times 10^{-27}}$$

$$\mu = 1.62 \times 10^{-27}\ \text{Kg.}$$

$$\Delta\bar{\nu} = \frac{h}{4\pi^2 I C} = 20.8 \times 10^2\ m^{-1}$$

$$\therefore \ I = \frac{6.654 \times 10^{-34}}{4\pi^2 \times 3 \times 10^8 \times 20.8 \times 10^2} = 2.689 \times 10^{-47}\ \text{Kg m}^2$$

$$r = \sqrt{\frac{I}{\mu}} = \sqrt{\frac{2.689 \times 10^{-47}}{1.62 \times 10^{-27}}} = 1.286 \times 10^{-10}\ m$$

3. Determine the rotational energy of CO on the quantum level $J = 2$ if the equilibrium nuclear distance of CO is 1.131 Å ($1 \text{ a.m.u} = 1.66 \times 10^{-27}$ Kg).

$$\text{Reduced mass } (\mu) = \frac{m_1 m_2}{m_1 + m_2} = \frac{16 \times 12}{16 + 12} = 6.857 \text{ a.m.u}$$

$$= 6.857 \times 1.66 \times 10^{-27}$$

$$\mu = 1.14 \times 10^{-26} \text{ Kg}$$

$$\text{Moment of Inertia } (I) = \mu r^2$$

$$I = 1.14 \times 10^{-26} \times (1.131 \times 10^{-10})^2$$

$$I = 1.46 \times 10^{-46} \text{ Kg m}^2$$

$$\text{Energy } (E) = \frac{h^2 J(J+1)}{8\pi^2 I}$$

$$E = \frac{(6.654 \times 10^{-34})^2 \times 6}{8\pi^2 \times 1.46 \times 10^{-46}} = 2.30 \times 10^{-22} \text{ J}$$

4. Find the energy and angular velocity of CO molecule in the ground state. Given CO bond length = 0.113 nm and mass of atoms $m_c = 1.99 \times 10^{-26}$ Kg and $m_o = 2.66 \times 10^{-26}$ Kg.

W.K.T Energy of diatomic molecule $= \dfrac{J(J+1) h^2}{8\pi^2 I}$

for ground state, $J = 0$

$$\therefore \quad E_J = 0$$

since energy $E_J = \frac{1}{2} I \omega^2$

$$\therefore \quad \frac{1}{2} I \omega^2 = 0$$

Angular velocity $(\omega) = 0$

5. In near IR spectrum of HCl molecule there is single intense band at 2885.9 cm^{-1}. Assuming that it is due to transition b/w vibration levels. Show that force constant K = 480 N/m.

Given :- $M_H = 1.68 \times 10^{-27}$ Kg

$$\because \quad \bar{\upsilon} = \frac{1}{\lambda} = \frac{\upsilon}{c}$$

$\therefore$ frequency of vibration $(\upsilon) = \bar{\upsilon} c = 288590 \times 3 \times 10^{8}$

$$\upsilon = 8.6577 \times 10^{13} \text{ Hz}$$

$$\because \quad \upsilon = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}} \quad \Rightarrow \quad K = 4\pi^2 \mu \upsilon^2$$

reduced mass $(\mu) = \dfrac{M_H M_{Cl}}{M_H + M_{Cl}} = \dfrac{1 \times 35}{(1+35)} \times M_H$

$$\mu = \frac{35 \times 1.68 \times 10^{-27}}{36} = 1.63 \times 10^{-27} \text{ Kg}$$

$$\therefore \quad K = 4\pi^2 \times 1.63 \times 10^{-27} \times (8.65 \times 10^{13})^2$$

$$K = 482.3 \text{ N/m.}$$

6. Calculate the vibrational energy levels of an HCl molecule, assuming the force constant to be 516 N/m.

Solution :- Reduced mass $(\mu) = \dfrac{35}{36} \times 1.0078 \times 1.66 \times 10^{-27}$

$$\mu = 1.62 \times 10^{-27} \text{ kg.}$$

$$\text{frequency } (\upsilon) = \frac{1}{2\pi}\sqrt{\frac{516}{1.62 \times 10^{-27}}}$$

$$\upsilon = 8.98 \times 10^{13} \text{ Hz}$$

Energy levels are given by $(\upsilon + \frac{1}{2}) h\upsilon$

$$\therefore \quad E_\upsilon = 6.654 \times 10^{-34} \times 8.98 \times 10^{13} \left(\upsilon + \tfrac{1}{2}\right) \text{ Joules.}$$

$$= 5.9 \times 10^{-20} \left(\upsilon + \tfrac{1}{2}\right) \text{ Joules}$$

for $\upsilon = 0$ $\quad E_{\upsilon=0} = 2.95 \times 10^{-20}$ J = 0.1843 ev

$\upsilon = 1$ $\quad E_{\upsilon=1} = 8.85 \times 10^{-20}$ J = 0.553 ev

$\upsilon = 2$ $\quad E_{\upsilon=2} = 14.75 \times 10^{-20}$ J = 0.921 ev

$\upsilon = 3$ $\quad E_{\upsilon=3} = 20.65 \times 10^{-20}$ J = 1.290 ev

7. The force Constant of CO bond is 187 Nm^{-1}. Find the frequency of Vibration of CO molecule. Given: Mass of $C^{12} = 1.99 \times 10^{-26}$ Kg and $O^{16} = 2.66 \times 10^{-26}$ Kg.

$$\text{Reduced mass } (\mu) = \frac{m_1 m_2}{m_1 + m_2}$$

$$\mu = \frac{1.99 \times 10^{-26} \times 2.66 \times 10^{-26}}{(1.99 + 2.66) \times 10^{-26}}$$

$$\mu = 1.14 \times 10^{-26} \text{ Kg}$$

$$\text{frequency of Vibration } (\nu) = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}}$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{187}{1.14 \times 10^{-26}}}$$

$$\nu = 2.04 \times 10^{12} \text{ Hz}$$

8. The ratio of population of two energy levels of which upper one Corresponds to a metastable state is 1.059×10^{-30}. Find the wavelength of emitted light at 330 K.

$$\text{Ratio of population } \frac{N_2}{N_1} = e^{-\frac{(E_2 - E_1)}{KT}}$$

$$1.059 \times 10^{-30} = e^{-\Delta E / 1.38 \times 10^{-23} \times 330}$$

$$\Delta E = 3.147 \times 10^{-19} \text{ J}$$

$$\text{Wavelength } (\lambda) = \frac{hc}{\Delta E}$$

$$\lambda = \frac{6.654 \times 10^{-34} \times 3 \times 10^{8}}{3.147 \times 10^{-19}}$$

$$\lambda = 632 \text{ nm}$$