

4) The spacing between two adjacent rotational lines in the rotational spectrum of the HCl molecule is $6.33 \times 10^{11} \text{ s}^{-1}$. Calculate the moment of inertia of the HCl molecule and the equilibrium internuclear distance if the molar masses are $1.008 \text{ gr mol}^{-1}$ for H and $34.97 \text{ gr mol}^{-1}$ for ^{35}Cl .

The rotational energy levels are given by:

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

The allowed transition is $\Delta J = \pm 1$, so for $J \rightarrow J-1$ transition we obtain:

$$\Delta E = E_J - E_{J-1} = \frac{J(J+1)h^2}{8\pi^2 I} - \frac{J(J-1)h^2}{8\pi^2 I} = \frac{h^2}{8\pi^2 I} [J(J+1 - J - 1)] = \frac{h^2 J}{4\pi^2 I}$$

The frequency emitted is:

$$\nu_J = \frac{\Delta E}{h} = \frac{hJ}{4\pi^2 I} = 2BJ \quad J = 1, 2, \dots$$

$$B \equiv \frac{h}{8\pi^2 I}$$

$$\Delta \nu = \nu_{J+1} - \nu_J = 2B(J+1) - 2BJ = 2B$$

So the spacing between frequencies is simply the rotational constant $2B$.

Now, for diatomic molecule the moment of inertia about the center of mass is:

$$I = \frac{m_1 m_2}{m_1 + m_2} R^2 = \mu R^2$$

Where μ is known as the reduced mass.

So we get:

$$\Delta \nu = 2B = \frac{h}{4\pi^2 I}$$

$$I = \frac{h}{4\pi^2 \Delta \nu}$$

$$R = \sqrt{\frac{h}{4\mu\pi^2 \Delta \nu}}$$

In our case (recall that the *gr/mol* unit is actually the definition of atomic mass unit) we obtain:

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{1.008 \times 34.97}{1.008 + 34.97} = 0.98 \text{ amu} = 0.98 \text{ amu} \times \frac{1.66 \times 10^{-27} \text{ kg}}{\text{amu}}$$

$$\mu = 0.162 \times 10^{-26} \text{ kg}$$

$$\Delta \nu = 6.33 \times 10^{11} \text{ s}^{-1}$$

$$h = 6.26 \times 10^{-34} \text{ m}^2 \cdot \text{kg} \cdot \text{s}^{-1}$$

$$R = \sqrt{\frac{h}{4\mu\pi^2 \Delta \nu}} = \sqrt{\frac{6.26 \times 10^{-34} \text{ m}^2 \cdot \text{kg} \cdot \text{s}^{-1}}{4\pi^2 \times (0.162 \times 10^{-26} \text{ kg}) \times (6.33 \times 10^{11} \text{ s}^{-1})}} = 0.124 \times 10^{-9} \text{ m}$$

So the bond length is 0.124 nm