SUBJECT - CHEMISTRY
CLASS - B.Sc (Hons) PART-III
PAPER — V
TOPIC — Vibrational-frequency of a diatomic molecule:

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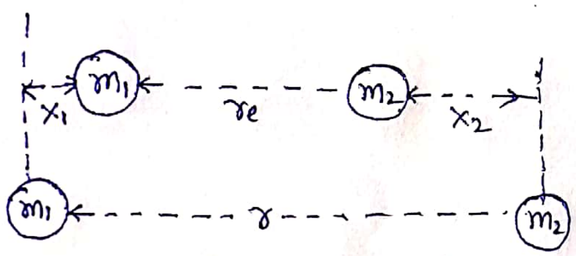
Q Express vibrational levels of a diatomic molecule in terms of the force Constant and masses of the atoms.

Vibrational-frequency of a diatomic molecule:

Let us Consider a diatomic molecule in which atoms having masses m_1 and m_2 oscillate against each other like a harmonic Oscillator.



Let r_e be the equilibrium distance between two atoms and r when stretched. Atoms Shift by $-x_1$ and x_2 in two opposite directions So that the displacement,

$$x = r - r_e = -x_1 + x_2 = x_2 - x_1$$

The restoring force on each atom is proportional to displacement x.

or Restoring force $= -K \cdot x$

where k = force Constant.

If x_1 and x_2 be the distances of the centre of gravity of the molecule from the centres of A and B atoms respectively then-

$$m_1 \frac{d^2 x_1}{dt^2} = -kx, \quad \text{or} \quad \frac{d^2 x_1}{dt^2} = -\frac{Kx}{m_1} \quad \text{---} \quad (i)$$

and $$m_2 \frac{d^2 x_2}{dt^2} = -kx, \quad \text{or} \quad \frac{d^2 x_2}{dt^2} = \frac{-kx}{m_2} \quad \text{---} \quad (ii)$$

$$\therefore \quad \frac{d^2(x_2 - x_1)}{dt^2} = -kx\left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

or $$\frac{d^2 x}{dt^2} = \frac{-kx}{\mu}, \quad \text{where } \mu = \text{reduced mass}$$

The Solution of this differential equation is given as

$$x = A \sin\sqrt{\frac{K}{\mu}} \cdot t + c \quad \text{---} \quad (iii)$$

The general equation of Simple harmonic motion is given as

$$x = A \sin 2\pi\nu \cdot t + c \quad \text{---} \quad (iv)$$

Comparing (iii) & (iv), we get

$$2\pi\nu = \sqrt{K/\mu} \quad \text{or} \quad \nu = \frac{1}{2\pi}\sqrt{K/\mu}$$

or $$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}} \quad \text{---} \quad (v)$$

Therefore, the vibrational frequency (ν) of a diatomic molecule is related to the force Constant (K) and reduced mass (μ).