SUBJECT - CHEMISTRY
CLASS - B.Sc (Hons) PART - III
PAPER - V
TOPIC - The vibrational frequency
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Q Show that the frequency of radiation absorbed by diatomic molecules behaving as harmonic oscillator is equal to its own oscillation frequency.

Ans. The vibrational frequency (ω) of a diatomic molecule behaving as harmonic oscillator is given as -

$$\omega = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \quad \text{--- (1)}$$

where k = force constant and μ = reduced mass

The restoring force may be taken as negative gradient of potential energy (V) as -

$$F = -kx = -\frac{\partial V}{\partial x}$$

$$\therefore \int dV = k\int_0^x x\,dx$$

$$\therefore V = k\left[\frac{x^2}{2}\right]_0^x = \frac{k}{2}\left[x^2\right]_0^x \quad \text{or, } V = \frac{1}{2}kx^2$$

The vibrational energy levels may now be determined from the following Schrodinger equation -

$$\nabla^2\psi + \frac{8\pi^2\mu}{h^2}\left[E - \frac{1}{2}kx^2\right]\psi = 0$$

The allowed solutions of this equation are given by -

$$E_{vib} = \frac{h}{2\pi}\sqrt{\frac{k}{\mu}}\left(v + \frac{1}{2}\right) \quad \text{--- (2)}$$

putting the value of ω from (1), we get

$$E_{vib} = \left(v + \frac{1}{2}\right) h\omega \quad \text{——— (3)}$$

where v is the vibrational quantum number having integral Values 0, 1, 2, 3, ---- Hence even at ground state i.e v = 0, The molecule would have vibrational energy $\frac{1}{2} h\omega$, Called Zero point energy. In vibrational transition from v to v′, the energy change is given by -

$$\Delta E = (v' - v) h\omega \quad \text{——— (4)}$$

for successive transition $v' - v = 1$, we have -

$$\Delta E = h\omega$$

$$\therefore h\nu = h\omega$$

$$\text{or } \nu = \omega$$

Therefore the frequency (ν) of the absorbed radiation by a diatomic molecule behaving as harmonic oscillator is equal to its own oscillation frequency (ω).