

# IR - Spectroscopy > Simple Harmonic Oscillator

Oscillation freq.

$$\omega_{osc} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \quad \text{Hz or } \bar{s}^{-1} \quad \text{--- (1)}$$

$$\bar{\omega}_{osc} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}} \quad \text{cm}^{-1} \quad \text{--- (2)}$$

$c \equiv \text{cm } \bar{s}^{-1}$  = speed of light

Vibrational energy for simple harmonic oscillator is

$$E_v = \left(v + \frac{1}{2}\right) h \omega_{osc} \quad \text{Joules} \quad \text{--- (3)}$$

$v = 0, 1, 2, \dots$

where,  $v$  is vibrational quantum number

$$\epsilon_v = \frac{E_v}{hc} \quad \text{cm}^{-1} \quad \therefore \text{Divide eqn (3) by } hc$$

$$\therefore \epsilon_v = \left(v + \frac{1}{2}\right) \bar{\omega}_{osc} \quad \text{cm}^{-1} \quad \text{--- (4)}$$

$\left(\because \bar{\omega}_{osc} = \frac{\omega_{osc}}{c}\right)$

For lowest vibrational energy level  
Put  $v=0$ , in

eq<sup>n</sup> (3) becomes

$$E_0 = \frac{1}{2} h \omega_{osc} \quad \text{joules} \leftarrow \underline{\underline{ZPE}}$$

eq<sup>n</sup> (4) becomes

$$E_0 = \frac{1}{2} \bar{\omega}_{osc} \quad \text{cm}^{-1} \leftarrow \underline{\underline{ZPE}}$$

ie in Ground state, diatomic molecule can never have zero vibrational energy

Selection rule for Harmonic Oscillator is

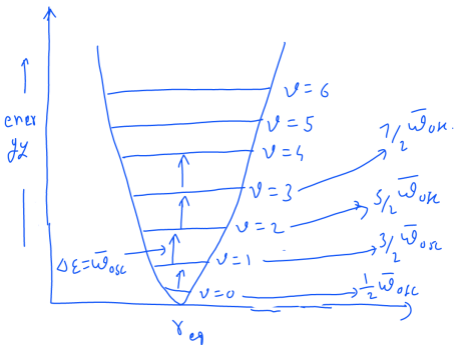
$$\Delta v = \pm 1$$

Condition for IR active: During vibration

there must occur change in Dipole moment. ie heteronuclear diatomic molecules are IR active

$$E_v = \left(v + \frac{1}{2}\right) \bar{\omega}_{osc}$$

Put  $v = 0, 1, 2, \dots$



Internuclear distance

Fig: vibrational energy levels and allowed transitions bet<sup>n</sup> them for a diatomic molecule undergoing simple harmonic motion.

Now apply a selection rule  
 i.e.  $\Delta v = \pm 1$ , i.e. transition takes place  
 from  $E_v$  to  $E_{v+1}$  state



$$\Delta E = E_{v+1} - E_v \quad \text{from eqn (4)}$$

$$\Delta E = \left(v + 1 + \frac{1}{2}\right) \bar{\omega}_{osc} - \left(v + \frac{1}{2}\right) \bar{\omega}_{osc}$$

$$\Delta E = E_{v+1 \rightarrow v} = \bar{\omega}_{osc} \text{ cm}^{-1}$$

↑  
for emission

$$\Delta E = E_{v \rightarrow v+1} = \bar{\omega}_{osc} \text{ cm}^{-1}$$

↑  
for absorption

i.e. vibrational energy levels are equally spaced

$$\therefore \bar{\nu}_{\text{spectroscopic}} = E = \bar{\omega}_{osc} \text{ cm}^{-1}$$