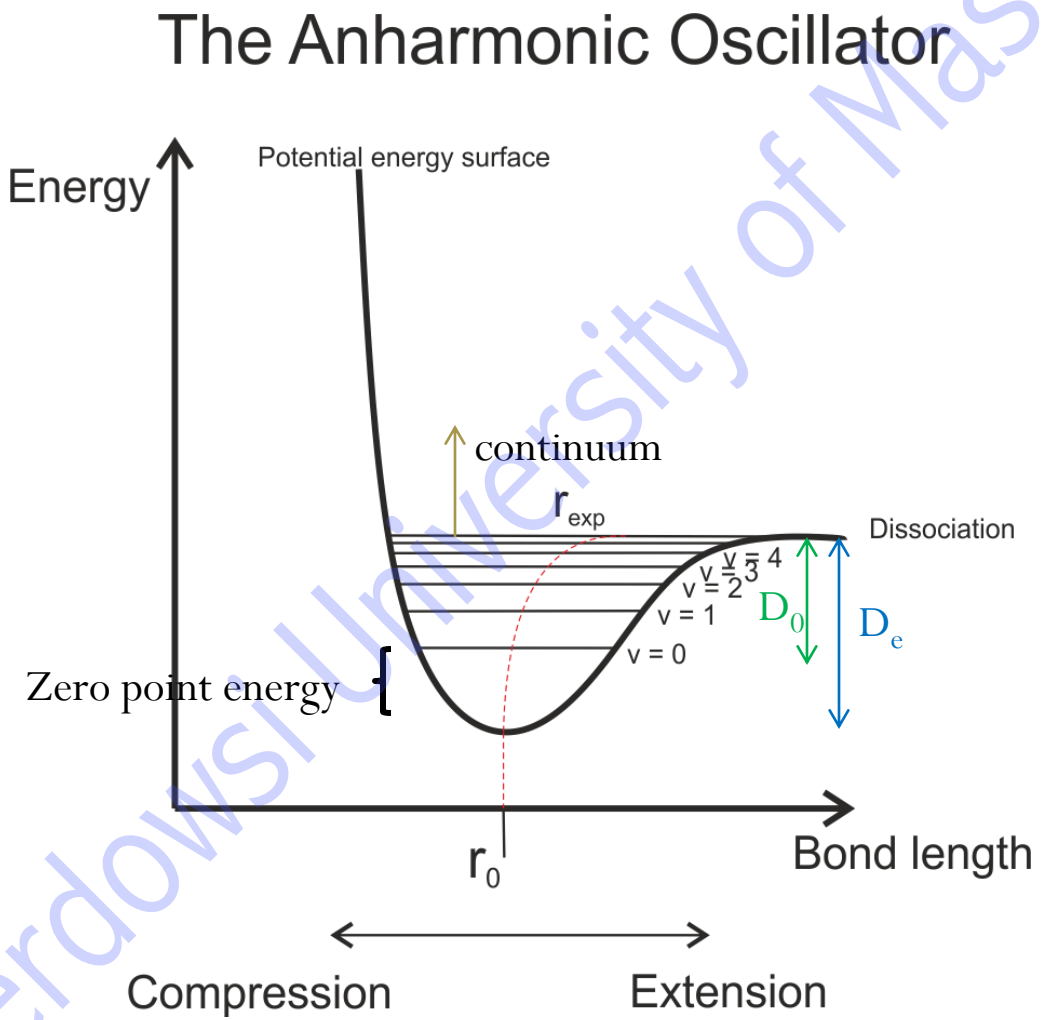
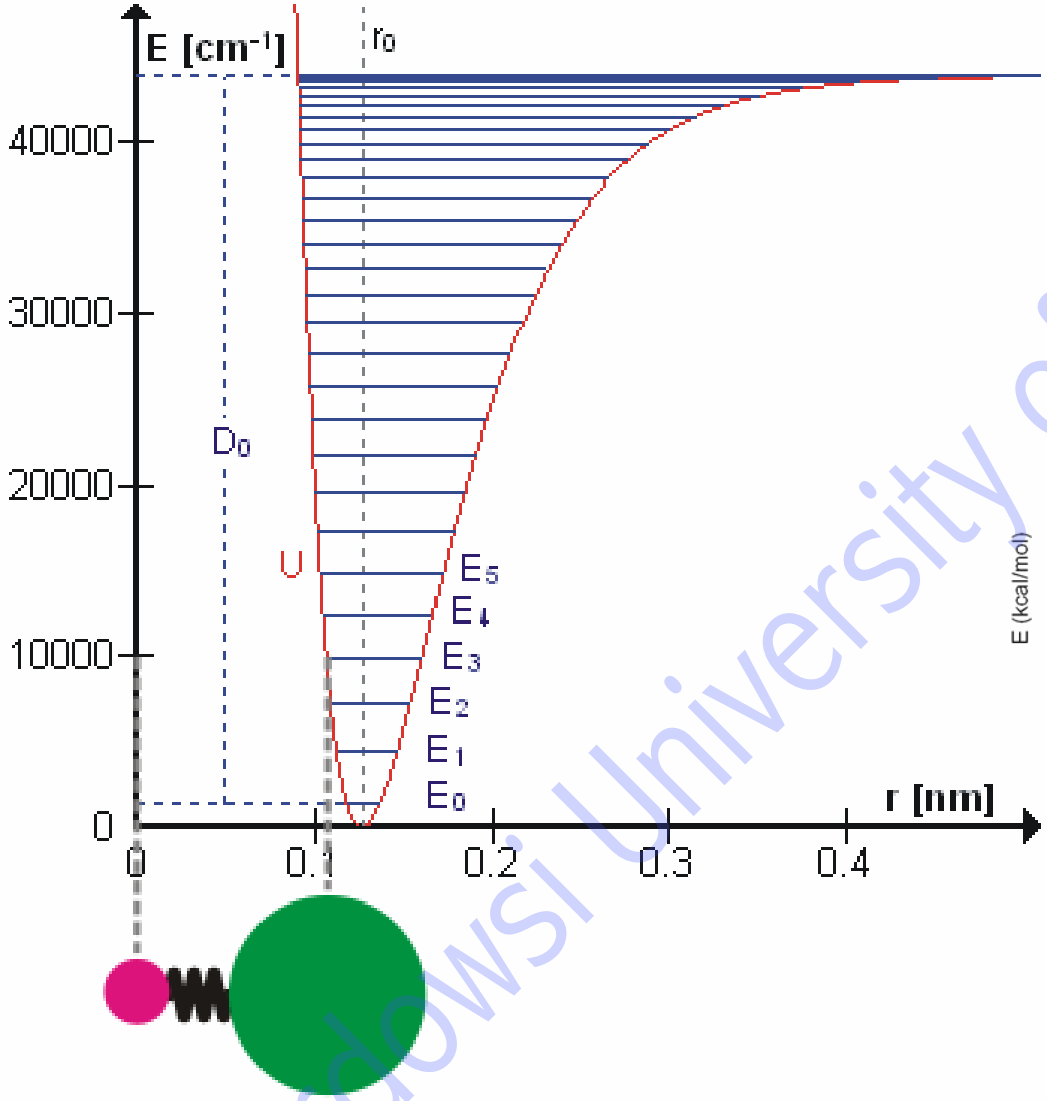
Spectroscopy in Inorganic Chemistry

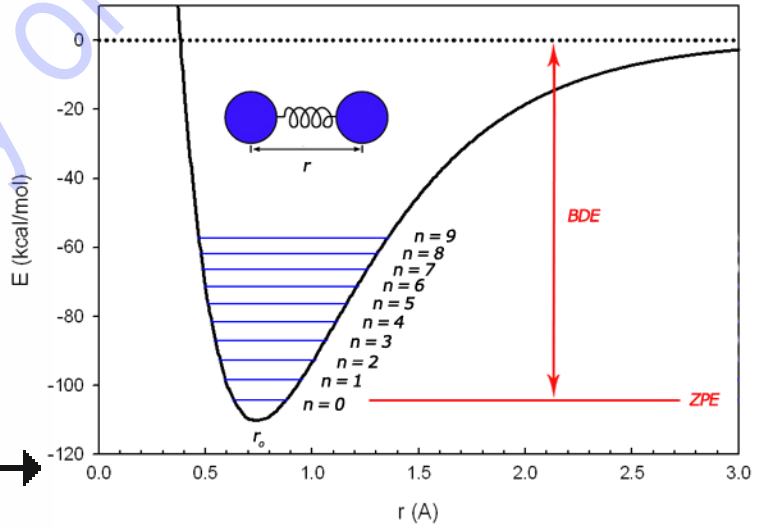
Electronic Absorption Spectroscopy

- Chapter 5 and 10

Vibrational and electronic energy levels in a diatomic molecule



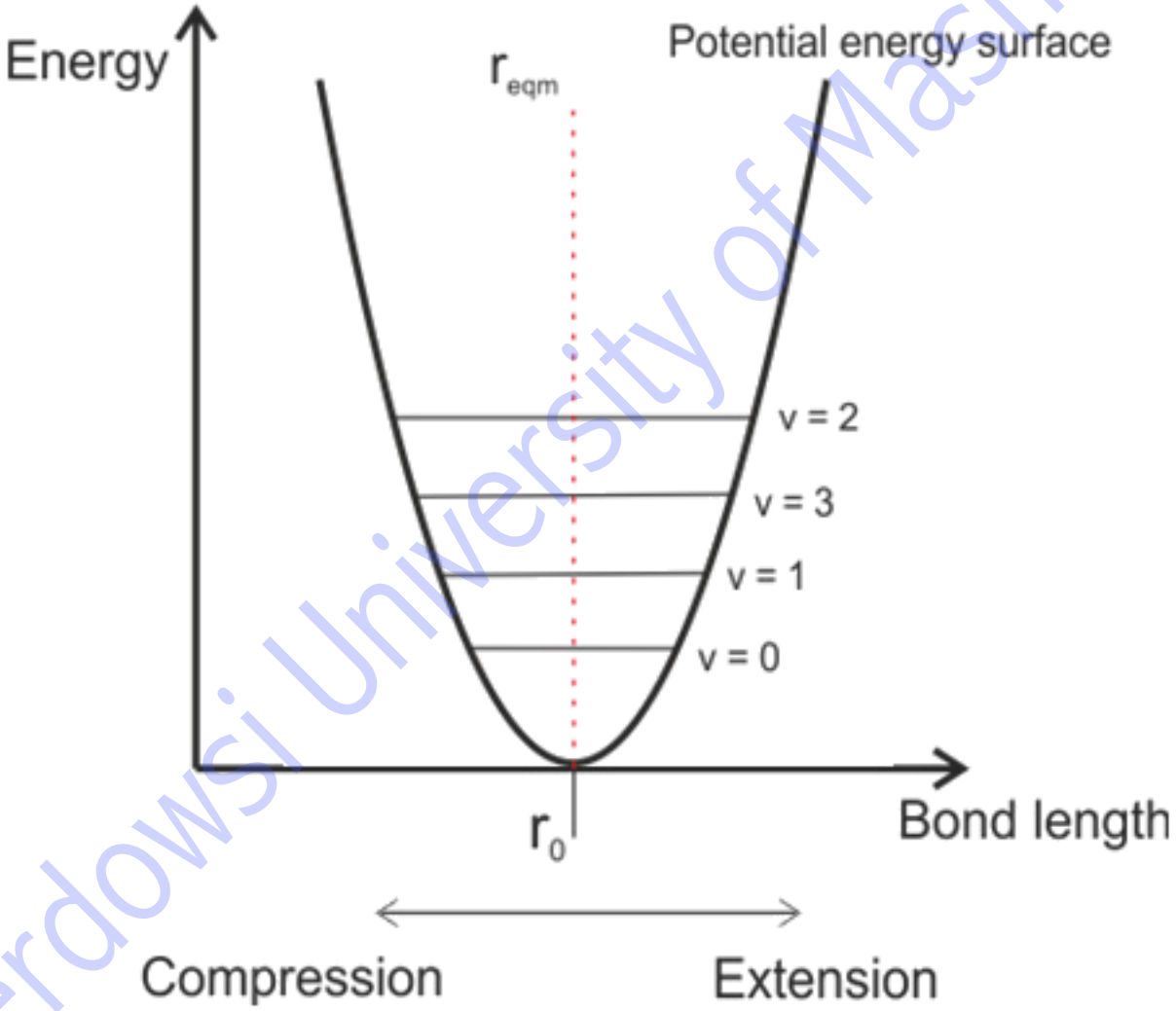




$$V = D\{1 - exp[-v_0(2\pi^2\mu D)^{1/2}(r - r_e)]\}^2$$

De

The Simple Harmonic Oscillator



$$E=\tfrac{1}{2}k(r-r_{eq})^2$$

$$\omega_{osc.} = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \quad \text{Hz}$$

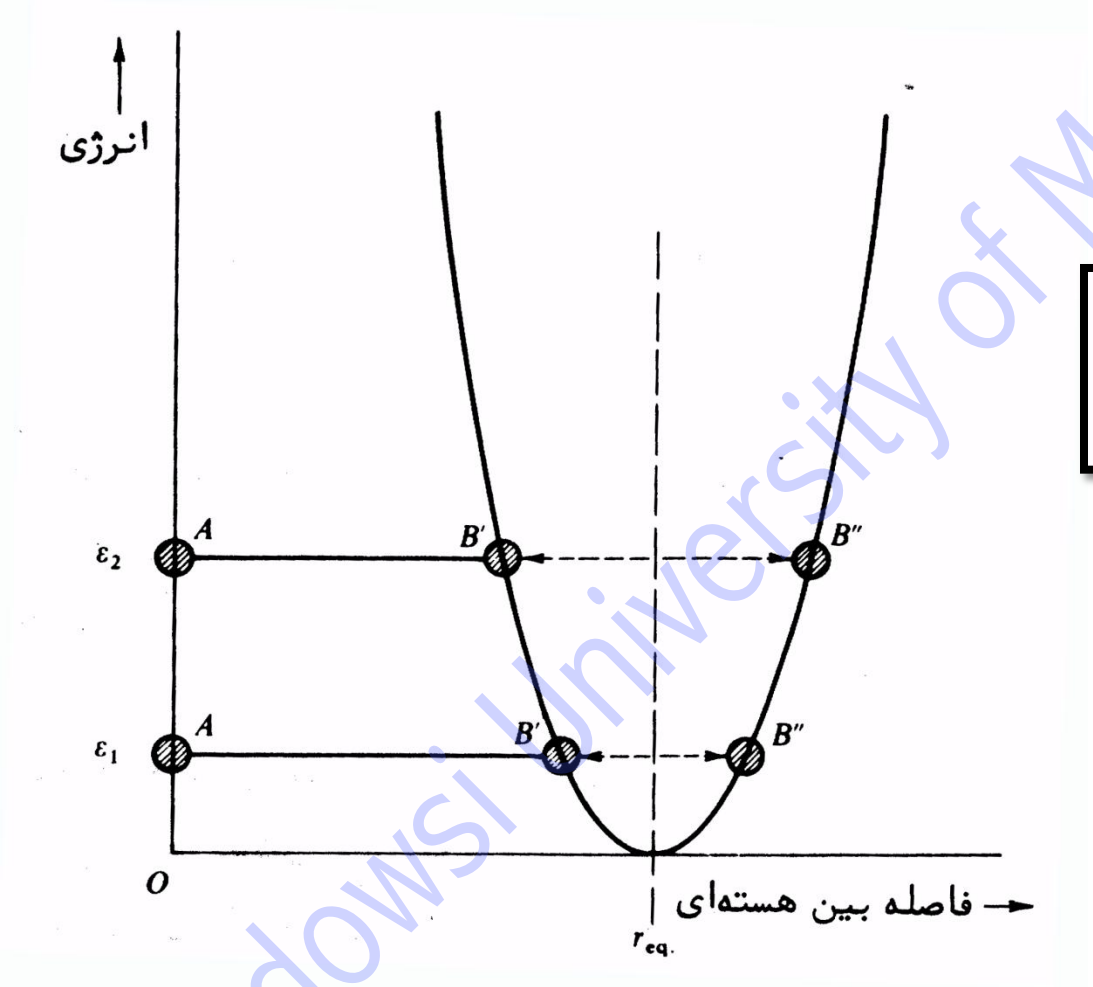
$$\bar{\omega}_{osc.} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} \quad \text{cm}^{-1}$$

$$E_v = (v + \tfrac{1}{2})h\omega_{osc.} \quad \text{joules} \qquad (v = 0, 1, 2, \ldots)$$

$$\varepsilon_v = \frac{E_v}{hc} = (v + \tfrac{1}{2})\bar{\omega}_{osc.} \quad \text{cm}^{-1}$$

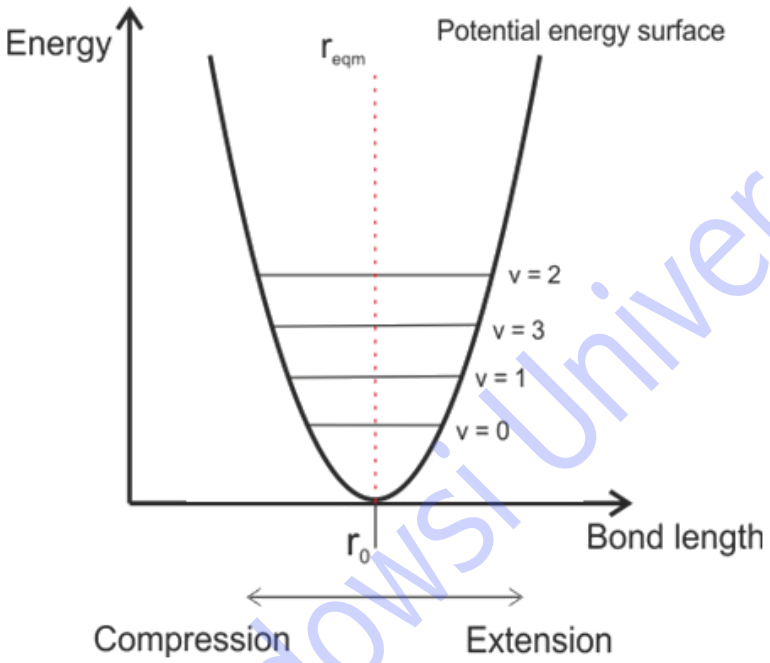
$$E_0 = \tfrac{1}{2}h\omega_{osc.} \quad \text{joules} \qquad [\text{Hz برحسب } \omega_{osc.}]$$

$$\varepsilon_0 = \tfrac{1}{2}\bar{\omega}_{osc.} \quad \text{cm}^{-1} \qquad [\text{cm}^{-1} \text{ برحسب } \bar{\omega}_{osc.}]$$

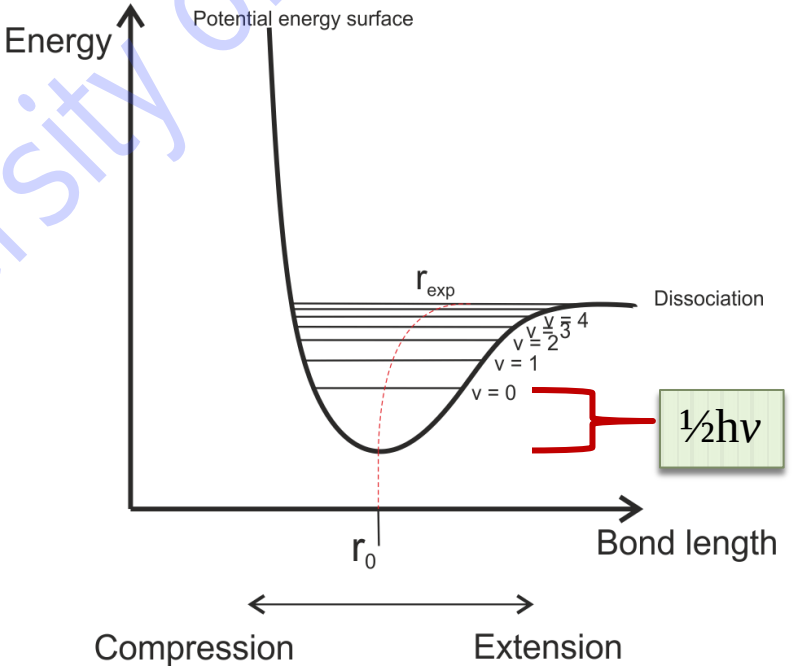


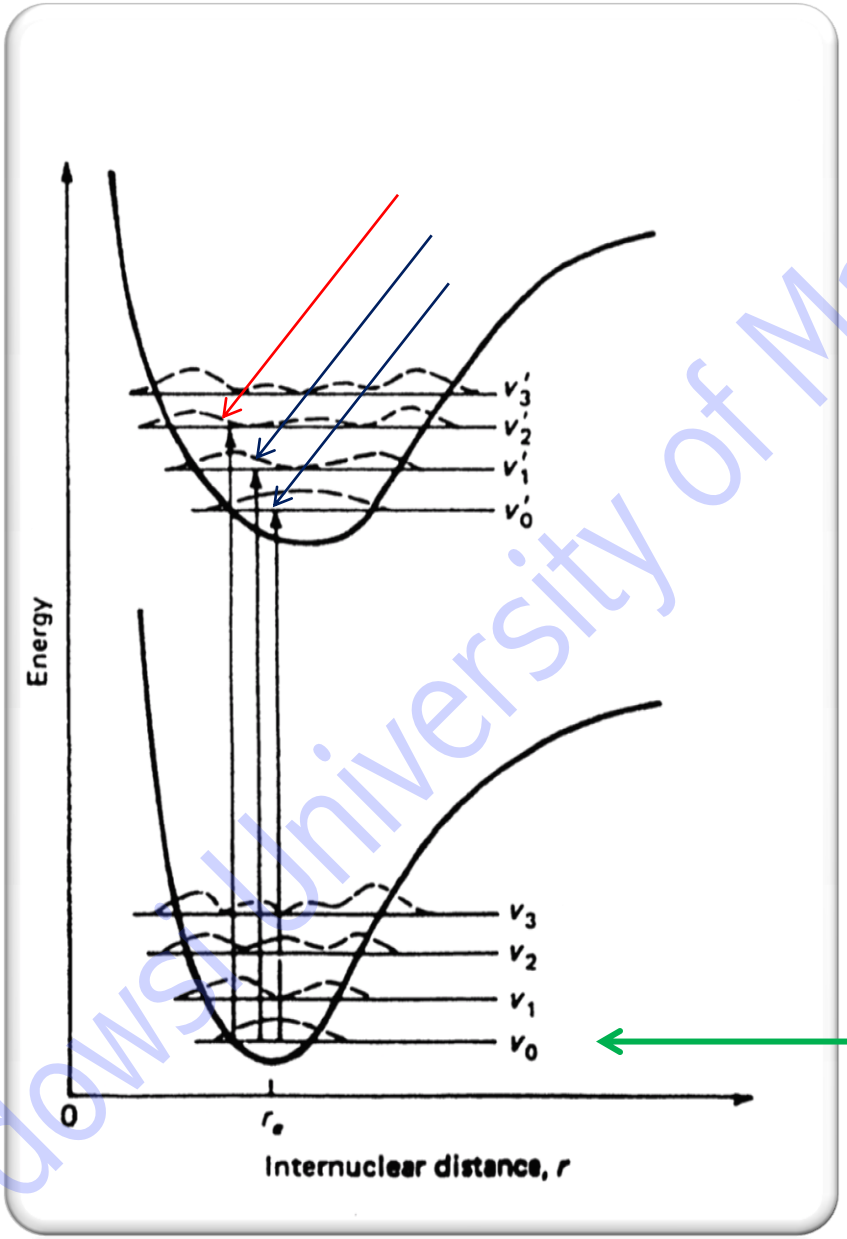
$$\bar{\omega}_{osc.} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} \quad cm^{-1}$$

The Simple Harmonic Oscillator



The Anharmonic Oscillator





Ψ_{vib}

Ψ^2_{vib}

Maximum population