

Absorption

$$A = [c] \epsilon l = -\ln\left(\frac{I_s}{I_r}\right)$$

$$A = -\ln T$$

T = transmittance

ϵ \equiv extinction coefficient

For systems in thermal equilibrium

The population ratio between E_f and E_i :

$$\frac{P(E_i)}{P(E_f)} = \frac{g(E_i)}{g(E_f)} \propto e^{-\frac{E_i - E_f}{k_B T}} \sim \propto e^{\frac{\Delta E}{k_B T}}$$

$$\Delta E = E_f - E_i$$

VIBRATIONS

Ollleed

$$F = -k(L - L_{eq})$$

$$x \equiv L - L_{eq}$$

$$V(x) = \frac{1}{2} k x^2$$

HARMONIC
OSCILLATOR

$$H\psi = -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} \psi + \frac{1}{2} k x^2 \psi$$

$$\Rightarrow \boxed{E_n = h\nu(n + 1/2)} \quad n=1, 2, 3, \dots$$

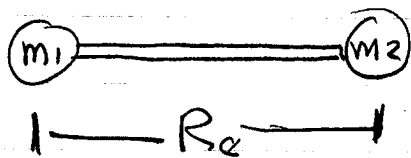
$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\boxed{E_{n+1} - E_n = h\nu} \quad \text{IR } (2-40) \text{ kJ mol}^{-1}$$

$$\text{Room Temp } k_B T \sim 2.5 \text{ kJ mol}^{-1}$$

ROTATIONS



$$I = \mu R_e^2$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

No radial dependence!

Classical $KE = \frac{1}{2I} L^2$

$h =$ angular momentum

Quantum U .

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

$$J = 0, 1, 2, 3, \dots$$

Selection Rule

$$\Delta J = \pm 1$$

$$E_{J+1} - E_J = 2 \left(\frac{h^2}{8\pi^2 I} \right) (J+1)$$

$$\nu = \frac{E_{J+1} - E_J}{h}$$

$$\nu = 2B(J+1)$$

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

ENERGY IN THE MICROWAVE REGION

Microwave ovens — 2.45 GHz (12.2 cm)

Radiation absorbed by water and small molecules with similar mass as water.

Metals reflect microwaves

Water absorbs — Rot ↑ and, through, collisions give up energy heating up the sample.

Microwave oven — 200–1000 W (TOTALLY SAFE)

Mobile phone — 1 W max (NOT CLEAR)