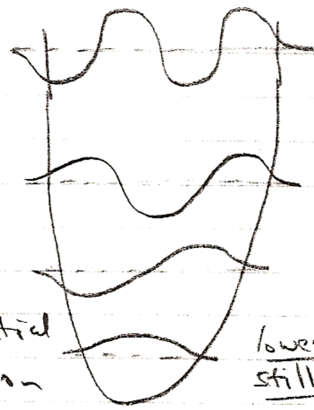
Vibration

implications $\psi_v(x)$



E_v	v	E_v
$\frac{7}{2}\hbar\omega$	3	$\frac{7}{2}h\nu$
$\frac{5}{2}\hbar\omega$	2	$\frac{5}{2}h\nu$
$\frac{3}{2}\hbar\omega$	1	$\frac{3}{2}h\nu$
$\frac{1}{2}\hbar\omega$	0	$\frac{1}{2}h\nu$
0		

lowest energy, still vibrates

* note like particle in box but can be found outside potential classically forbidden region

observe some tunnelling since potential not = ∞
boundary conditions cause energy to be quantized

$$E_v = (v+\tfrac{1}{2})\hbar\omega \qquad \omega = \sqrt{\frac{k}{m}}$$

force const / mass

$$E_v = (v+\tfrac{1}{2})\frac{h}{2\pi}\sqrt{\frac{k}{m}}$$

What you need to remember

$$\boxed{E_v = (v+\tfrac{1}{2})h\nu} \quad \text{where } \boxed{\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}}$$

$$\boxed{\nu = \frac{\omega}{2\pi}}$$

don't need ~~not~~ most of 14.2

$v = 0, 1, 2 \ldots$ → what we normally refer to as frequency

Implications:

~~for~~ molecular bonds

vibrational frequency $\nu \simeq 10^{14}\,s^{-1} \rightarrow 10^{13}$

$$\Delta E = h\nu = N_A h\nu = \quad N_A h\nu = (6.63\times10^{-34}\,J\,s)(6.02\times10^{23})(10^{14}\,s^{-1})$$

for 1 mole

$= 39912\ J \quad 39\ kJ$ — Significant chemical bonds ~100 kJ

$$\nu\lambda = c \qquad \frac{\nu}{c} = \frac{1}{\lambda} \qquad \frac{10^{14}\,s^{-1}}{3\times10^{8}\,m\,s^{-1}} \times \frac{m}{10^{2}\,cm} = 3333\ cm^{-1}$$

size of energy gap	$\nu\ (s^{-1})$	$1/\lambda\ (cm^{-1})$ reciprocal wavenumbers
40 kJ/mol	10^{14}	$3333\ cm^{-1}$
4 kJ/mol	10^{13}	$333\ cm^{-1}$

Infrared Radiation

Vibrational Spectroscopy

Thermal Energy not enough to break bonds

$$\Delta E = \frac{3}{2}RT = \frac{3}{2}\left(8.31\,\frac{J}{mol\,K}\right)(298\,K) = 3715\ J$$

3.7 kJ

get chart