# Ch 12 Infrared spectroscopy / Mass spectrometry

Note Title 10/10/2005

Lab reports due in class Wednesday: - salicylic acid
- stereochemistry

Infrared radiation longer wavelengths than visible light

gamma X-ray UV visible light IR microwaves radio

shorter ← wavelength → longer

this frequency causes bonds to vibrate

$\lambda$ = wavelength
(lambda)

inversely proportional

$\nu$ = frequency
(nu)

$c = \lambda \nu$

IR radiation $\lambda = 2.5 \times 10^{-4}$ cm to $2.5 \times 10^{-3}$ cm

c = speed of light

$\bar{\nu}$ = wavenumber $= \frac{1}{\lambda}$ units = $\text{cm}^{-1}$ (reciprocal centimeters)
(nu-bar)

measurement ~~unit~~ for IR radiation

convert to $\bar{\nu}$

$$\underbrace{\bar{\nu} = \frac{1}{\lambda}} = \frac{1}{2.5 \times 10^{-4}\ \text{cm}} = 4000\ \text{cm}^{-1}$$

$$\frac{1}{2.5 \times 10^{-3}\ \text{cm}} = 400\ \text{cm}^{-1}$$

standard range of IR radiation

$$\lambda = \frac{1}{\bar{\nu}}$$

$$c = \lambda \nu = c = \frac{\overset{\text{freq}}{\nu}}{\underset{\text{wavenumber}}{\bar{\nu}}} \qquad \bar{\nu} = \frac{\nu}{c}$$

wavenumber is proportional to frequency!

"fast" vibration = high wavenumber

slow = low $\bar{\nu}$

$E = h\nu$ $\qquad \bar{\nu} = \frac{\nu}{c} \quad = \quad \bar{\nu} = \frac{E}{hc}$

Planck's constant

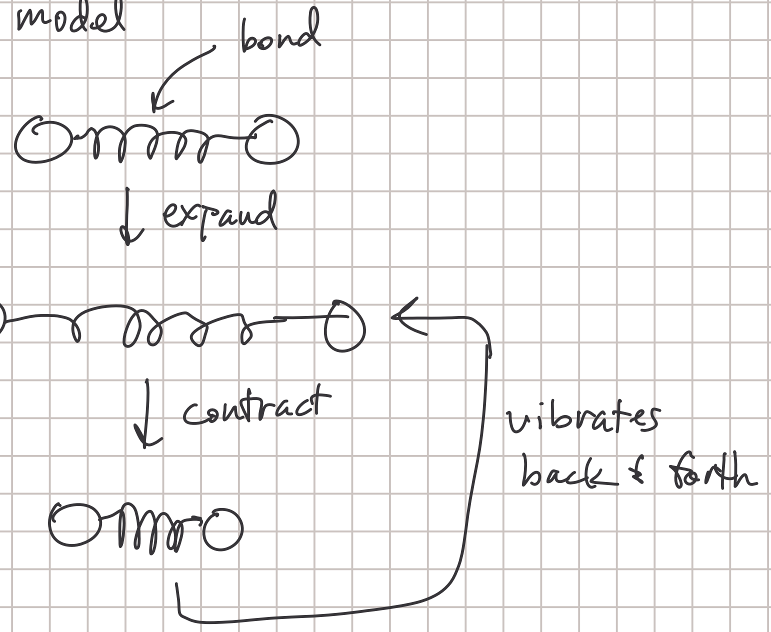
$\nu = \frac{E}{h}$

wave number is proportional to Energy as well

high $\bar{\nu}$ = high energy & vice/versa

Covalent bonds vibrate with a characteristic frequency

ball & spring model



different types of bonds vibrate faster than others.

"resonant frequency"

★ heavier atoms vibrate more slowly (low freq = low $\bar{\nu}$)

heavier ↓

slower vibration ↓

| | $\bar{\nu}$ ($cm^{-1}$) |
|---|---|
| C—H | 3000 |
| C—D | 2100 |
| C—C | 1200 |

## Stronger bonds vibrate faster

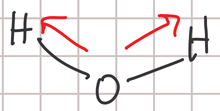
| | $\bar{\nu}$ (cm$^{-1}$) |
|---|---|
| C—C | 1200 |
| C=C | 1660 |
| C≡C | 2200 |

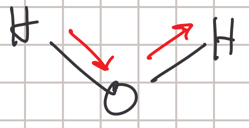
stronger ↓

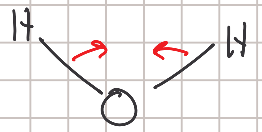
faster vibrations (tighter) ↓

increasing $\bar{\nu}$ ↓

## vibrational modes

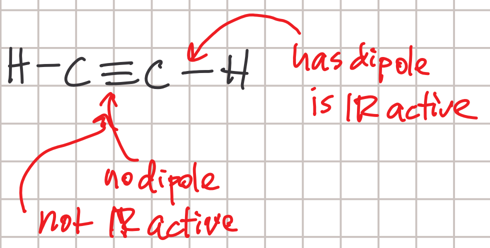

symmetric stretch (both bonds expand at same time) and then contract

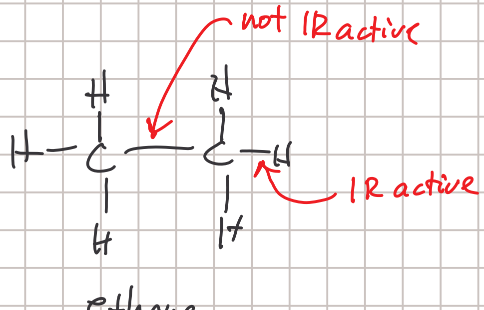

asymmetric stretch


bend

## IR-active bonds

only vibrations that cause a net dipole change are IR active

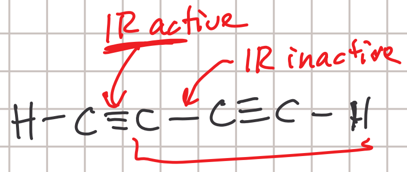




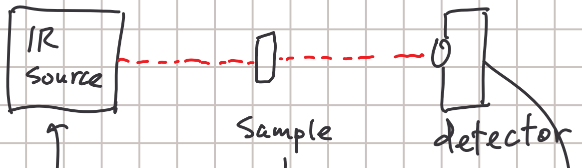
ethane

any bond made of 2 different atoms is always IR active

a bond made of 2 of the same atom is IR inactive IF both sides of molecule are identical as well



# IR spectrometer



all IR frequencies

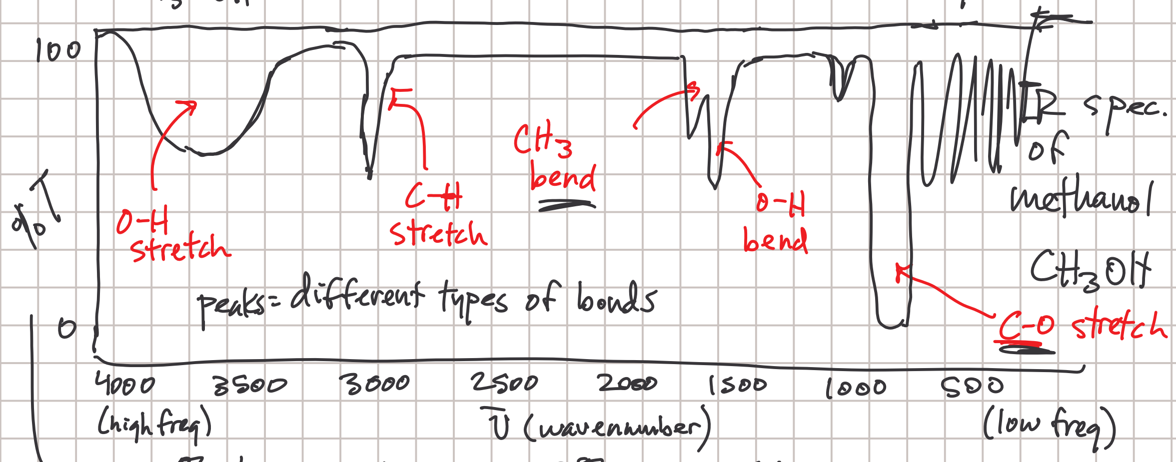
may absorb some IR frequencies (based on types of bonds)

detector measures which IR frequencies are diminished or missing

→ computer

$CH_3-OH$

IR spectrum



% transmittance 0% — 100%

↳ all light received by detector (none absorbed by sample)

→ no light received (all absorbed)