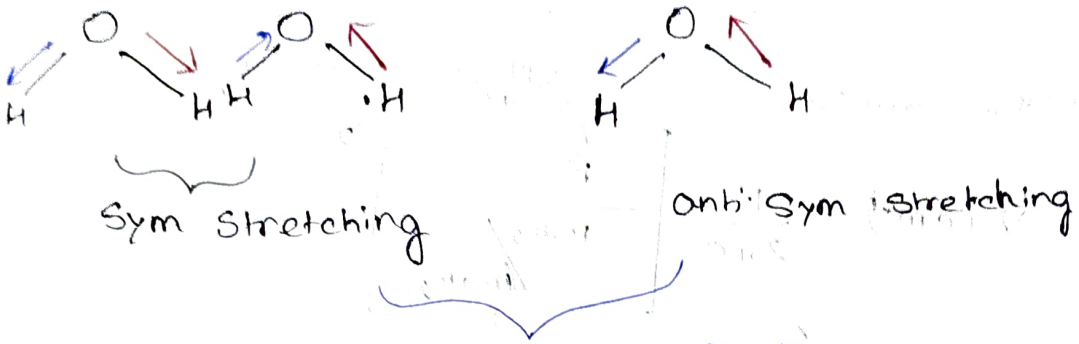
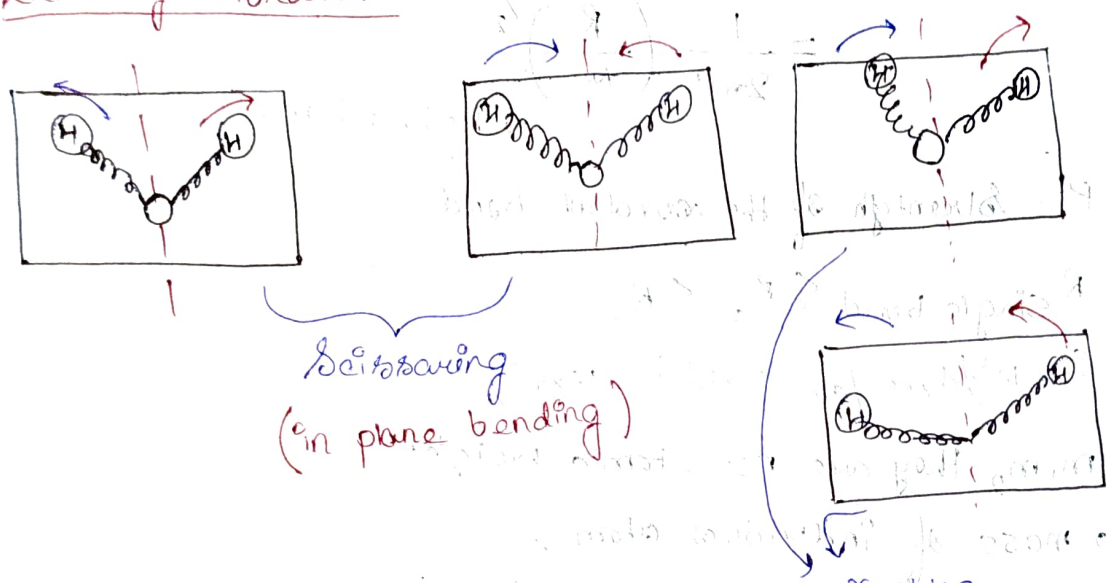
Spectroscopy

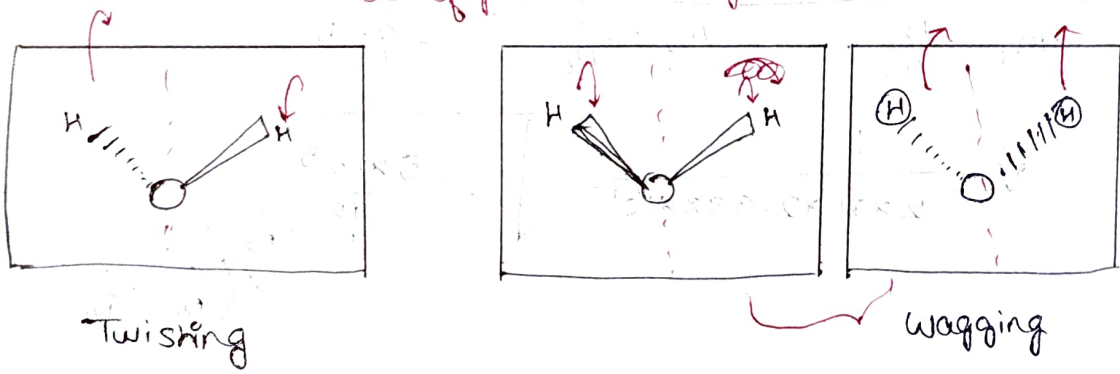
Types of vibrations in a molecule

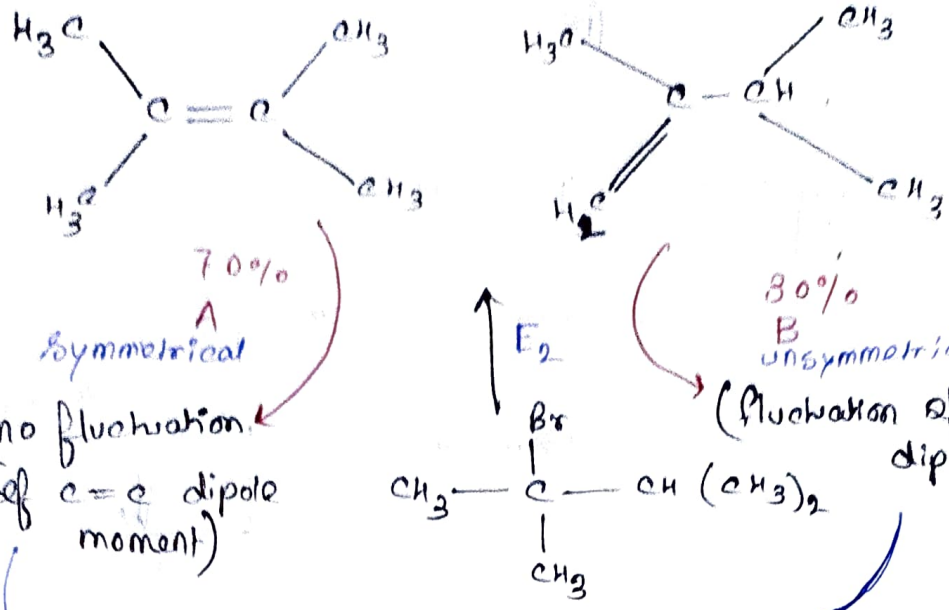
example ⇒ H_2O (triatomic, non linear)



Bending Vibration:







$\bar{\nu}_{c=c} \approx 1620 - 1680\ cm^{-1}$

no sp^2 c-H bond

sp^2 CH bond ($\bar{\nu} \approx 3100\ cm^{-1}$)

* 1. A ⇒ no signal at 1620-1680 cm^{-1} ($\bar{\nu}_{c=c}$)

2. B ⇒ no signal at 3100 cm^{-1} ($\bar{\nu}_{sp^2 c-H}$)

problem

$$\bar{\nu}_{O-H} > \bar{\nu}_{O-D} \quad \text{or} \quad \bar{\nu}_{OH} < \bar{\nu}_{OD}$$

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{R}{\mu}}$$

The mass of D = 2 × mass of H atom (μ) dominant

$$\mu_{OD} \geq \mu_{OH} \quad (R)$$

$$\bar{\nu}_{O-H} \geq \bar{\nu}_{O-D}$$

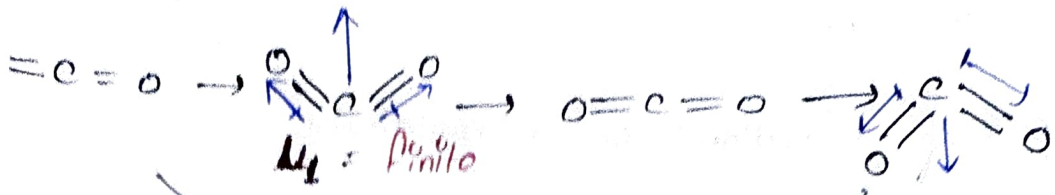
Correlation Table ⇒

Alcohols, phenols ⇒ OH ⇒ 3200 cm^{-1} - 3600 cm^{-1}

Amines ⇒ N-H ⇒ (3000 - 3200) cm^{-1}

carboxylic acid ⇒ $-\overset{\overset{O}{\|}}{C}-O-H$ ⇒ (2500) cm^{-1}

aldehyde ⇒ $\overset{\overset{O}{\|}}{C}-H$ ⇒ 1720 cm^{-1}



fluctuation of dipole moment ⟶ CO_2 IR active

How to cal the fre of vib

Hook's Law ⇒

$$\bar{\nu}\ (cm^{-1}) = \frac{1}{2\pi c}\left[\frac{R}{m_1 m_2/(m_1+m_2)}\right]^{1/2}$$

R ← Stiffness of the string

c ← velocity of light

m_1, m_2 ← mass of the balls

$$= \frac{1}{2\pi c}\left(\frac{R}{\mu}\right)^{1/2}$$

μ ← reduced mass

R = Strength of the covalent bond

$R_{\text{Single bond}} < R_= < R_\equiv$

(5×10^5) dynes/cm (10×10^5) (15×10^5)

m_1, m_2 they are not atomic weight

↳ mass of individual atom.

For Sp^3 C-H Bond

$$m_1 = \frac{12}{N_0} \qquad m_2 = \frac{1}{N_0} \qquad -\overset{1}{\underset{1}{C}}-H$$

$$\bar{\nu} = \frac{1}{2\times\pi\times2.998\times10^{10}}\sqrt{\frac{5\times10^5}{\frac{12}{N_0}\times\frac{1}{N_0}\Big/\left(\frac{12}{N_0}+\frac{1}{N_0}\right)}}$$

$$= 3032\ cm^{-1}$$

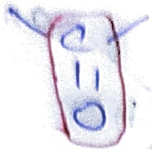
for Sp^2 C-H

$\bar{\nu}\ (cm^{-1}) = 3100\ cm^{-1}$ $=C-H$

for Sp C-H

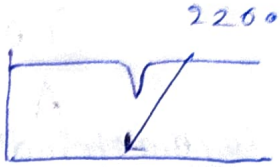
$\approx 3300\ cm^{-1}$

$\equiv C-H$

Ketone ⇒  ⇒ (1700 - 1710) cm^{-1}

Amide ⇒  ⇒ (1680) cm^{-1}

$C \equiv C$ ⇒ (2100 - 2200) cm^{-1}



$C \equiv N$ ~ 2200 cm^{-1}