Chapter:

Molecular Spectroscopy

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Infrared Spectroscopy
(IR)

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Chemistry with MJS

IR- Spectroscopy

→ vibrational spectroscopy

IR Region

Near IR	M- IR	Far- IR
0.8 – 2.5 μm	2.5 – 15 μm	15 – 200 μm
12500 /14000 – 4000 cm^{-1}	4000 – 400/667 cm^{-1}	667/400 – 50/10 cm^{-1}

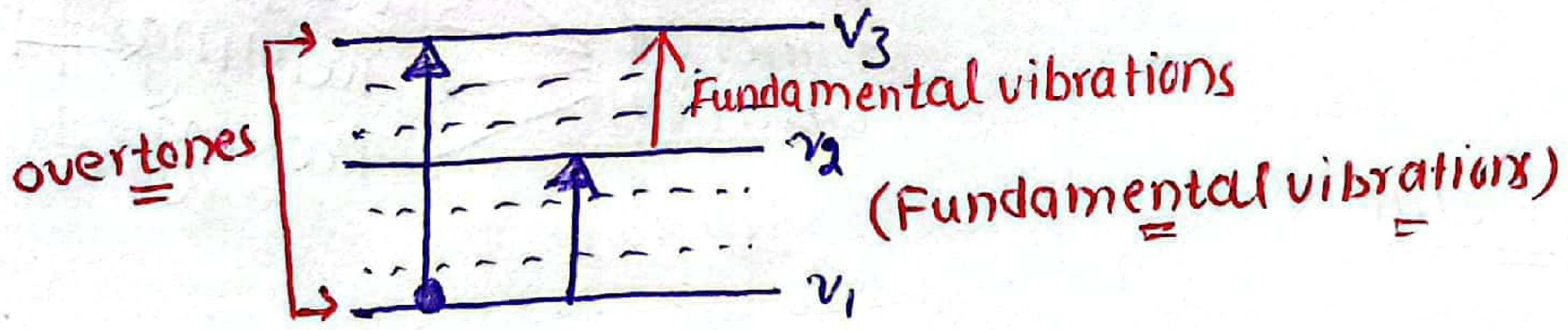
conversion $1 \mu m =$ ____ cm^{-1} ?

$cm =$ ____ cm^{-1}

$\therefore \lambda \propto \frac{1}{\bar{\nu}}$

principle:

IR ⟶ Absorbed by molecules
↓
excitation of molecules From lower to higher vibrational levels.



IR- Active / Inactive compounds:

Dipole moment imp. Factor For IR Absorption

★ $\mu = 0 \Rightarrow$ IR inactive compound → Not IR absorbed
↓
Not molecular Absorptions

e.g $H_2, N_2, O_2, Cl_2,$ etc.

★ $\mu =$ ..... IR active compounds

All types of complex organic compounds show IR- Absorption.

→ Degree of Freedom

vibrations are the degree of freedom

↓

Modes of vibrations

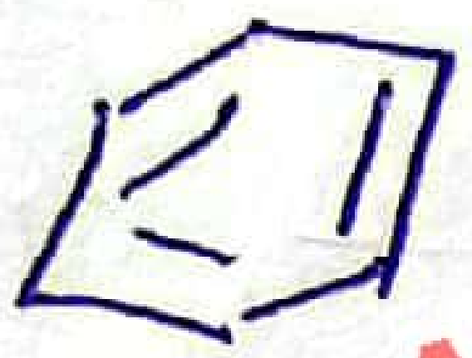
- tranlational
- Rotational
- vibrational

★ For linear Molecules ⇒ $3n-5$ e.g CO_2 ($3\times3-5 = 4$ vibrations)

★ For Non-linear molecules ⇒ $3n-6$ e. H_2O $3\times3-6 = 3$ vibrations

↓

maximum peaks for H_2O are 3

e.g Benzene 

$3(12)-6 = 30$ vibrations → weak signals

↓

closely spaced

↓

merged.

Vibrational Modes: (Fundamental vibrations)

two main modes of Fundamental

- Stretching vibrations
  - Symmetric
  - Asymmetric
- Bending
  - vibrations
    - Scizzoring (inplane)
    - Wagging (out of plane)
    - Twisting (out of plane)
    - Rocking (inplane)

Stretching:

↳ Movement of two bonded Atoms along the bond axis & interatomic distance increasing or decreasing.

$\overleftarrow{O} = C = \overrightarrow{O}$

symmetric stretching

$\overrightarrow{O} = \overrightarrow{C} = O$

Asymmetric /Antisymmetric stretching.

∴ $\nu_{stretching} > \nu_{Bending}$

∴ $\nu_{Asymm} > \nu_{symmetric}$

Bending:

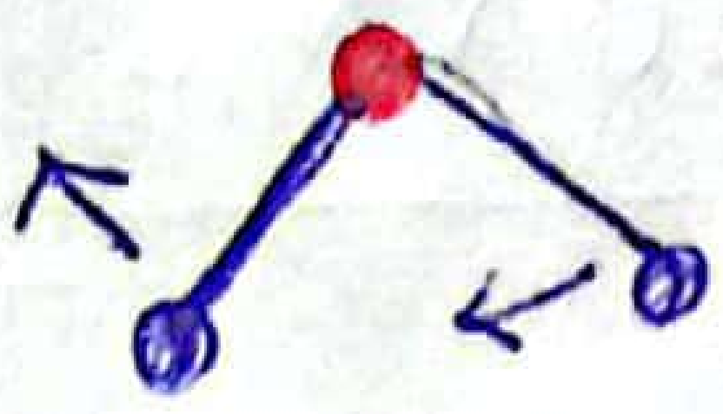
★ change in the angle b/w bonds with a common Atom but interatomic distance does not change.

→ For Bending → 3 Atoms Required.

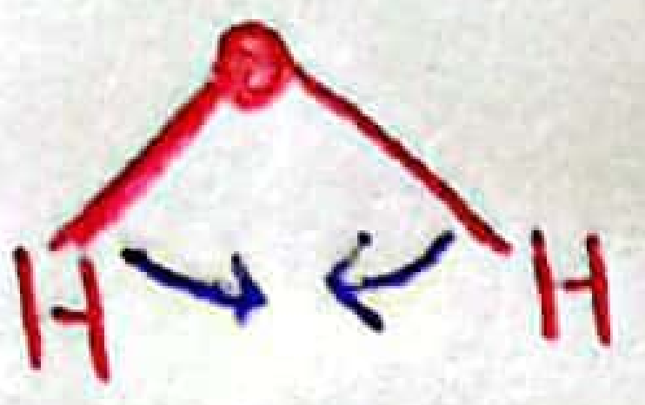
(SR)

Scissoring

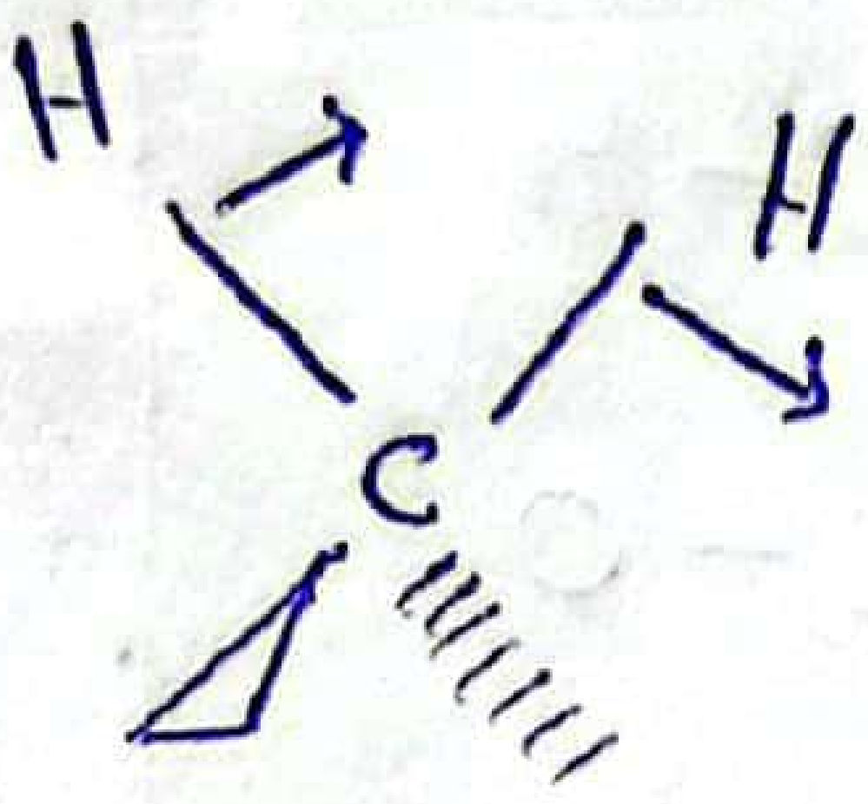
Rocking →



In plane



two atoms approach eachother)

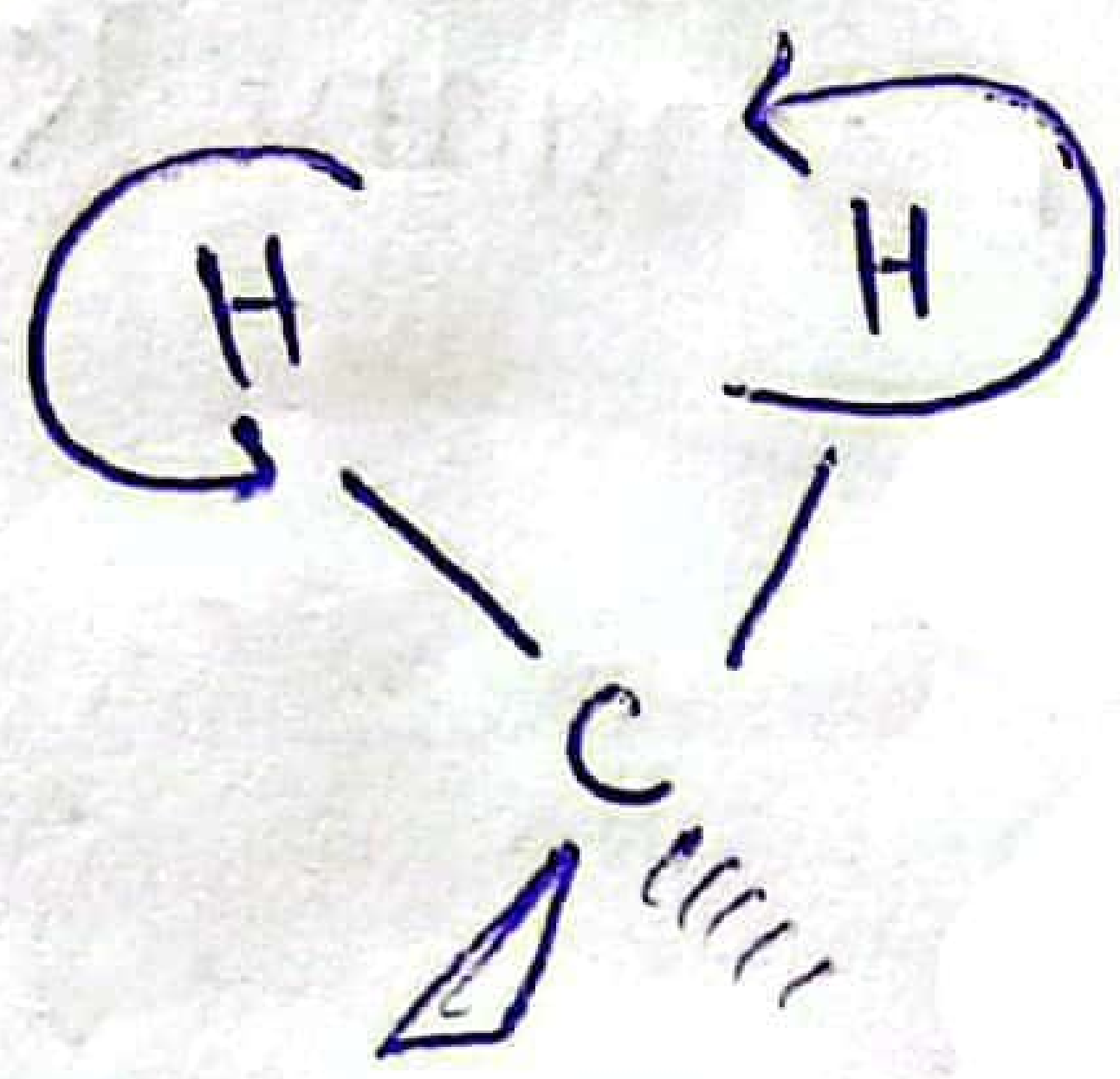


Movement of Atoms (in same direction) in same plane

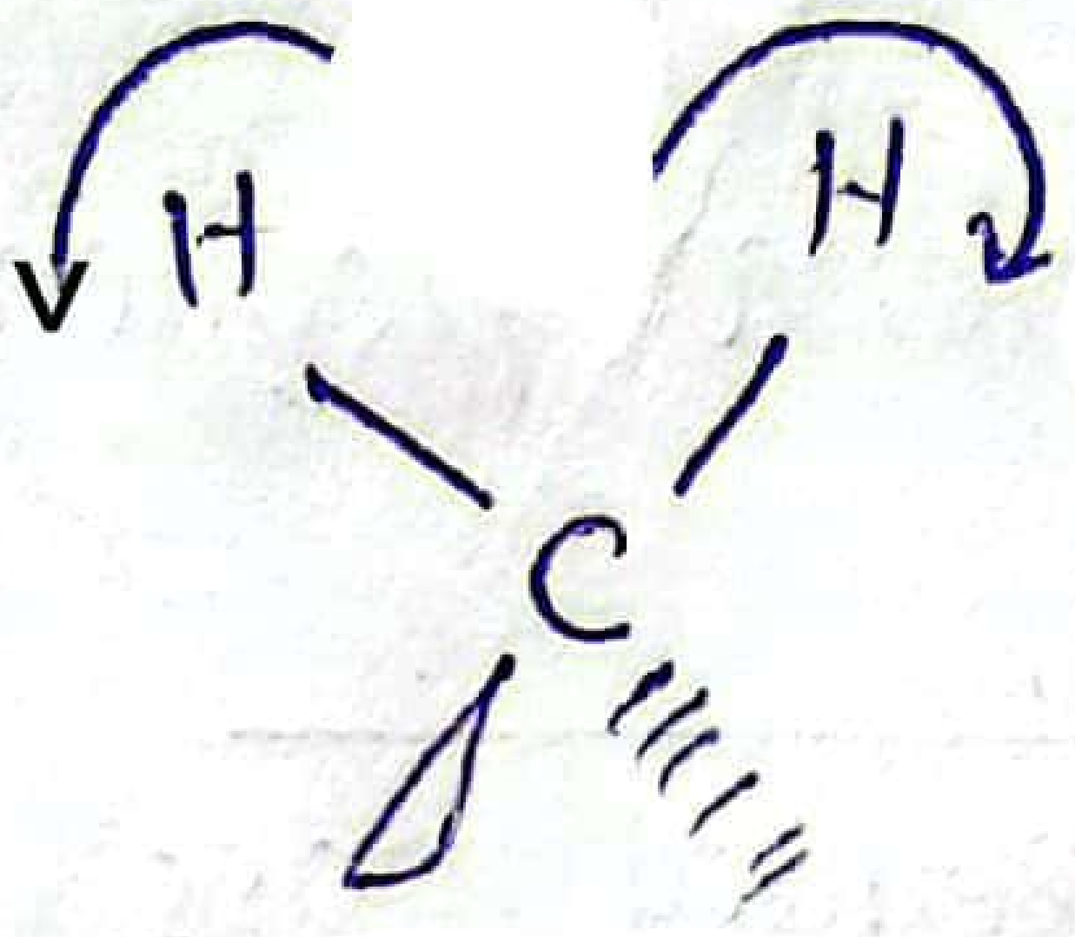
out of plane

one move up the plan (towards us) & other move down the plane ↓ far from us

Twistting



wagging → Both two atoms Simultaneous movement up & down out plane ↓ simultaneousley both comming toward us or going Far us



✓ vibrational Frequency (ν) (HOOK's Law)

vibration of Bonds are just like HOOK's Law ↓ spring system

✓ It depends upon two factors

(i) Bond strength (K)

(ii) Reduced mass (μ)

(vib. Freq) $\nu = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}}$ ⇒ $\mu = \frac{m_1 m_2}{m_1 + m_2}$ = (amu)

∴ 1 amu = 1.66×10^{-27} kg

∴ 1 amu = 1.66×10^{-24} g

(wave number) $\bar{\nu} = \frac{1}{2\pi C}\sqrt{\frac{K}{\mu}}$

C ↓ $3 \times 10^{10}\ cm\,s^{-1}$

∴ If K ⇒ N/m Then use kg unit of Reduced Mass

∴ If K ⇒ dyn/cm Then use g (μ)

C–O, O–H, N–H, C–C, C=C, C≡C, C–H

C≡N,

∴ O–H ⇒ $\frac{16 \times 1}{16+1} = \frac{16}{17} =$

∴ Reduced Mass

∴ N–H ⇒ $\frac{14 \times 1}{14+1} = \frac{14}{15} =$

∴ C–C ⇒ $\frac{12 \times 12}{12+12} =$

∴ C–O ⇒ $\frac{12 \times 16}{12+16} =$

∴ $\boxed{1\ \text{dyn/cm} = 1000 \times \text{N/m}}$

Example;

Calculate the vibrational frequency & wave no. of OH bond whose Strength K = 770 N/m

Bonds	K
O−H	770 N/m
C−O	1860 N/m
C−H	5×10^5 dyn/cm
C=C	10×10^5 dyn cm⁻¹

(i) ν (vibrational frequency) $\propto$ Bond constant K

(ii) $\nu \propto \dfrac{1}{\text{Reduced mass}}$.

Regions

4 Regions

① H-bond Region (Lighter Region) ⟶ (4000 − 2200 cm⁻¹)

② Triple Bond Region ⟶ (2200 − 2000 cm⁻¹)

③ Double bond Region ⟶ (1800 − 1550 cm⁻¹)

④ Finger print Region ⟶ (1500 − 650 cm⁻¹)

Factors Affecting Absorption frequency / vibrational Frequency / wave Number:

① Nature of Bond:

Bond strength is defined by the nature of Bond either single, Double or Triple.

$\bar{\nu}$ (cm⁻¹) $\quad \underset{\sim 2150\ \text{cm}^{-1}}{\overset{}{C\equiv C}} > \underset{\sim 1650\ \text{cm}^{-1}}{C=C} > \underset{\sim 1200}{C-C}$

$\overset{sp^2}{>C=N}$ ≈ 1650 cm⁻¹

$\overset{sp}{C\equiv N}$ ≈ 2250 cm⁻¹

$\overset{sp^3}{C-N}$ ≈ 1350−1000 cm⁻¹

② Hybridisation:

sp^3, sp^2, sp

Higher will be the s-character → higher will be the electronegativity, then higher will be the Bond strength.

$\bar{\nu} \Rightarrow sp > sp^2 > sp^3$

$\therefore \underset{sp^3}{C-O} \longrightarrow 1300-1000\ cm^{-1}$

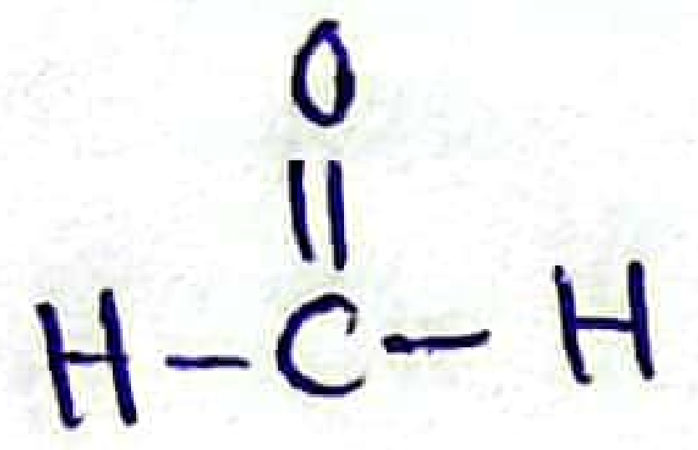
$\therefore \underset{sp^2}{C=O} \longrightarrow 1600-1750/1800\ cm^{-1}$

③ Electronic Effects:

Absorption frequency can be changed due to the substituent in the neighbourhood of the particular group. ⋆ Inductive Effect: (Distance Effect)

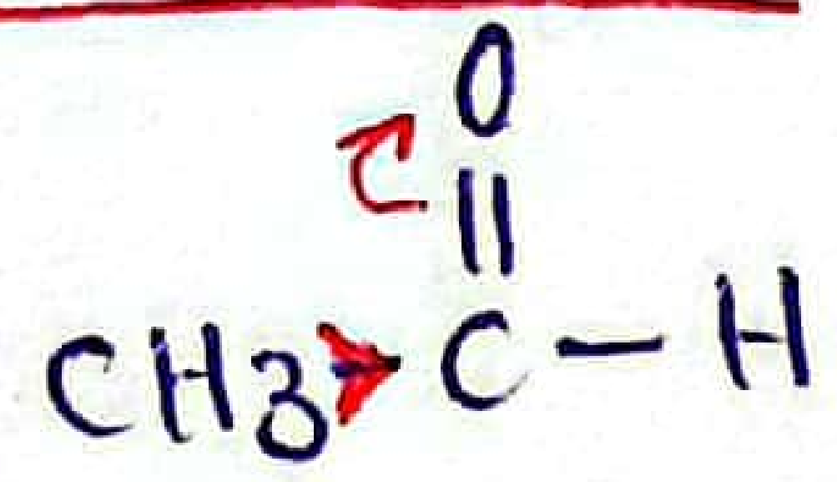
⇒ Effects May be inductive Effect | Mesomeric Effect

⋆ +I increase the length of bond → thus strength decreases thus Absorption frequency decreases.



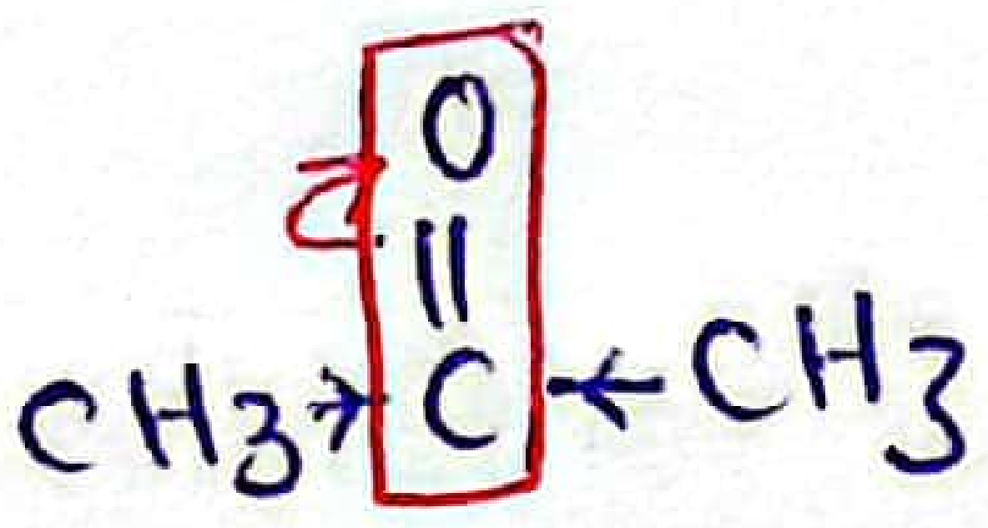
$H-\overset{O}{\overset{\|}{C}}-H$

1750 cm^{-1}



$CH_3 \rightarrow \overset{O}{\overset{\|}{C}}-H$

≈ 1725 cm^{-1}



$CH_3 \rightarrow \overset{O}{\overset{\|}{C}} \leftarrow CH_3$

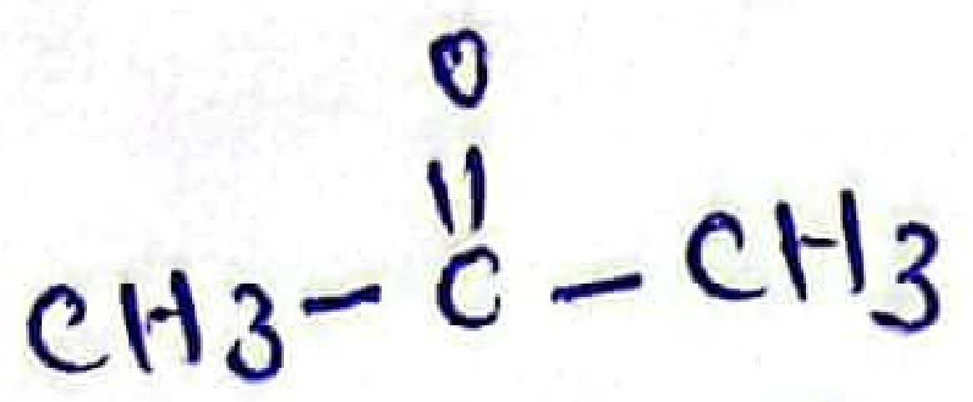
≈ 1715 cm^{-1}

⋆ in case of ketone Bond more elongates than Aldehyde thus Absorption frequency decreases

→ Attachment of ē-N atom → which decrease the Effect of conjugation/elongation

⋆ −I Effect increase the wave number value B/c of increase of bond order.

e.g

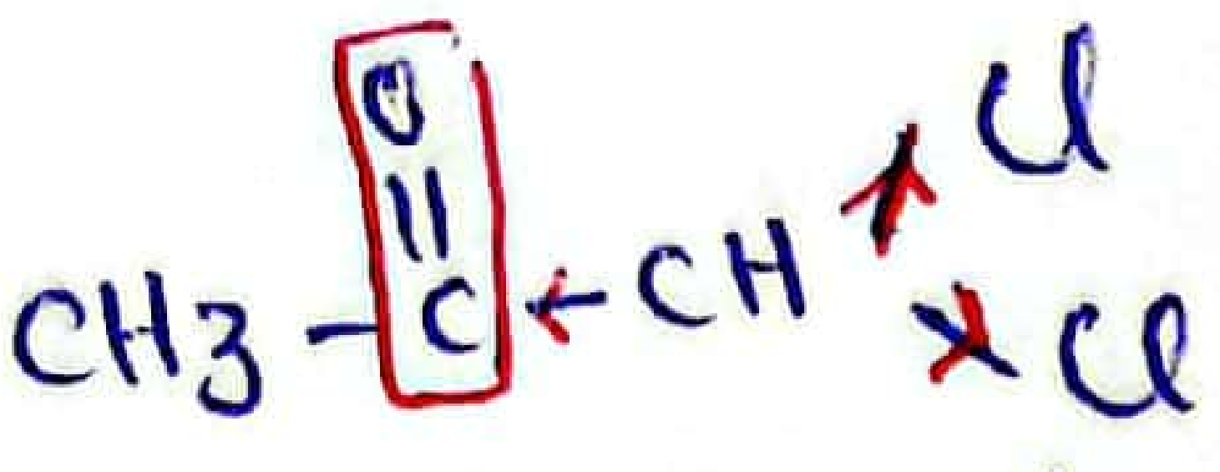


$CH_3-\overset{O}{\overset{\|}{C}}-CH_3$

1715 cm^{-1}

$CH_3-\overset{O}{\overset{\|}{C}} \leftarrow CH_2 \rightarrow Cl$

1725 cm^{-1}



$CH_3-\overset{O}{\overset{\|}{C}} \leftarrow CH \begin{smallmatrix} \nearrow Cl \\ \searrow Cl \end{smallmatrix}$

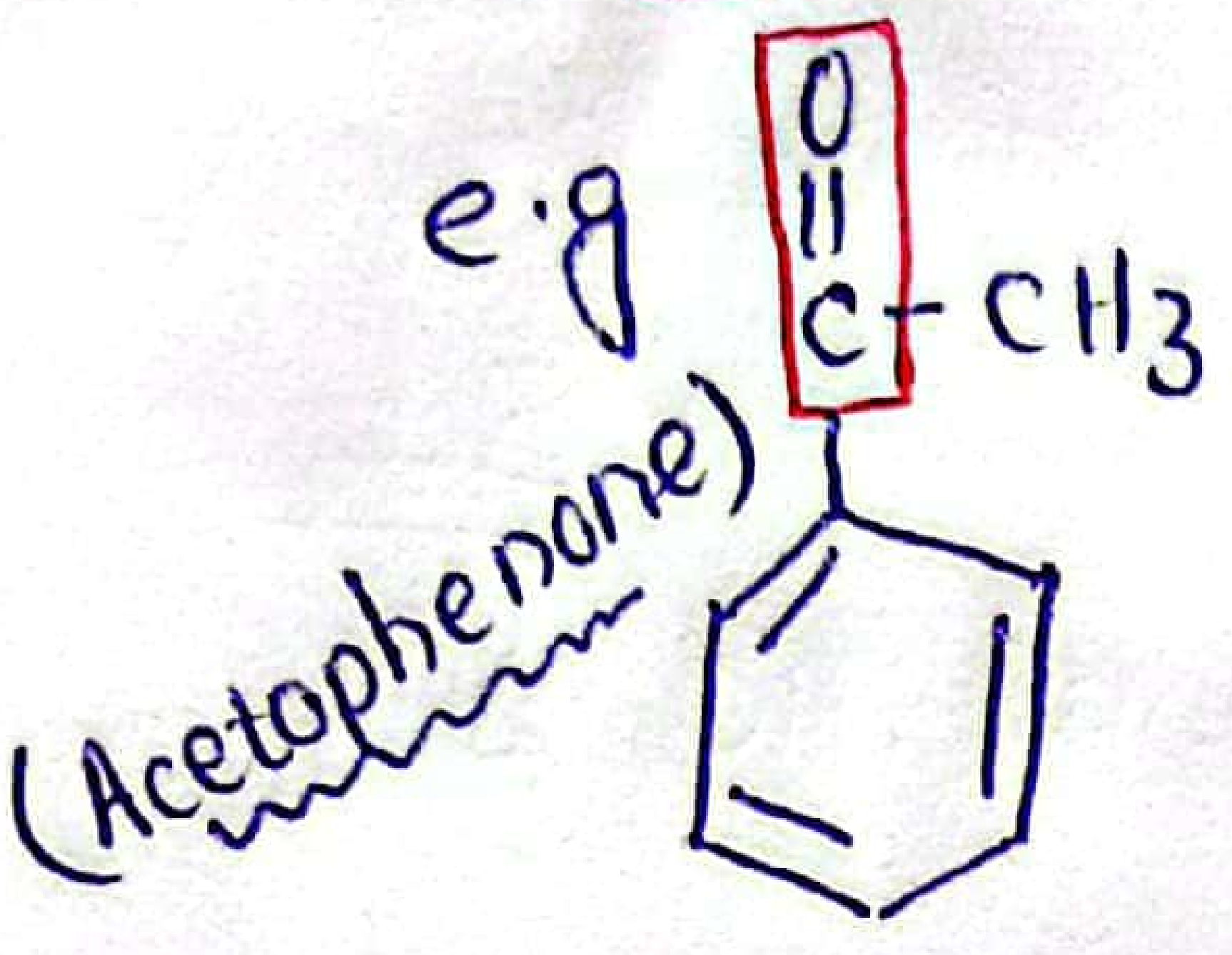
1740 cm^{-1}

Mesomeric Effect | Resonance

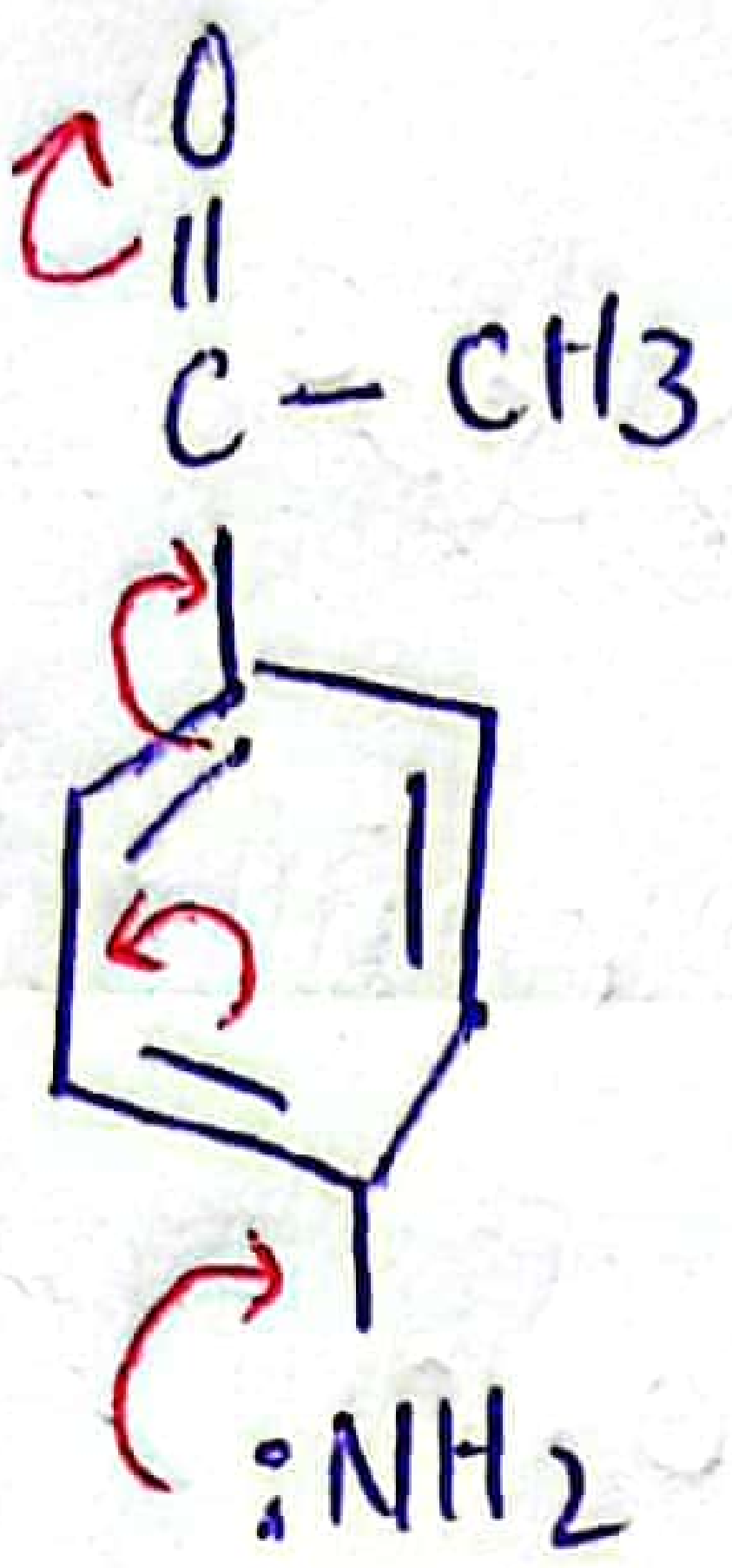
★ +M → increase the conjugation in the Ring → thus elongate the C=O thus wavenumber derease

★ −M → NO elongation of C=O → increase wavenumber

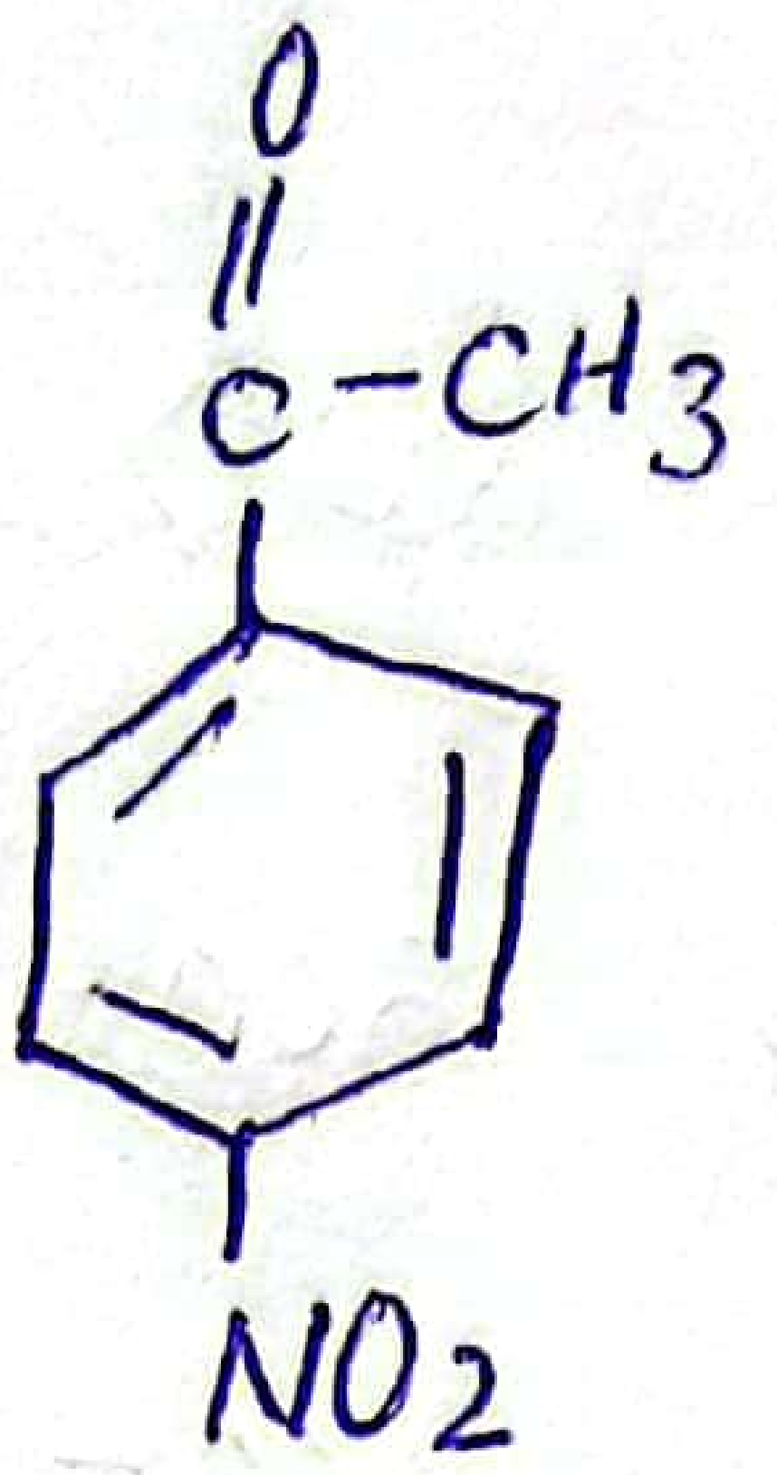
e.g



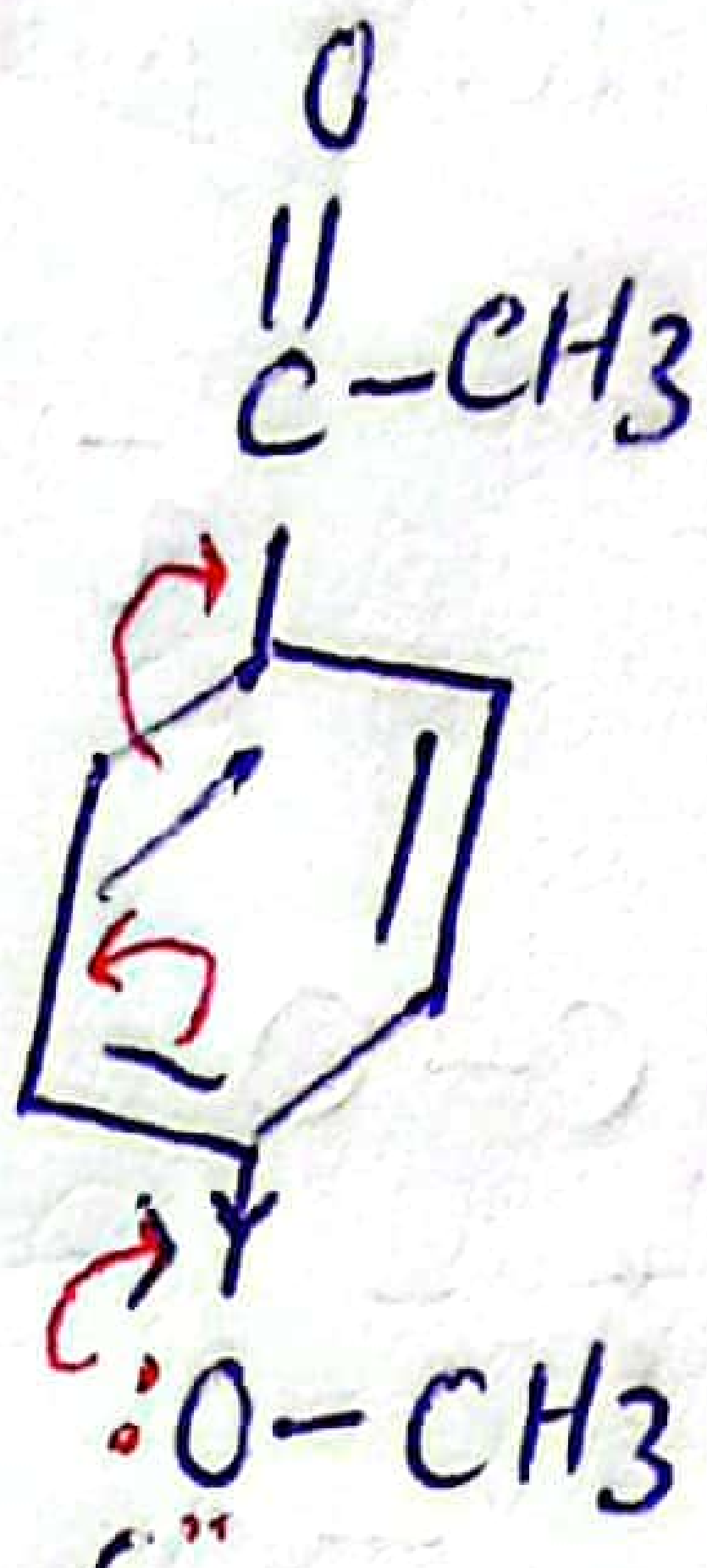
1693 cm⁻¹



1670 cm⁻¹



1700 cm⁻¹



more E.N
↓
Thus show the −I- Effect

1685 cm⁻¹

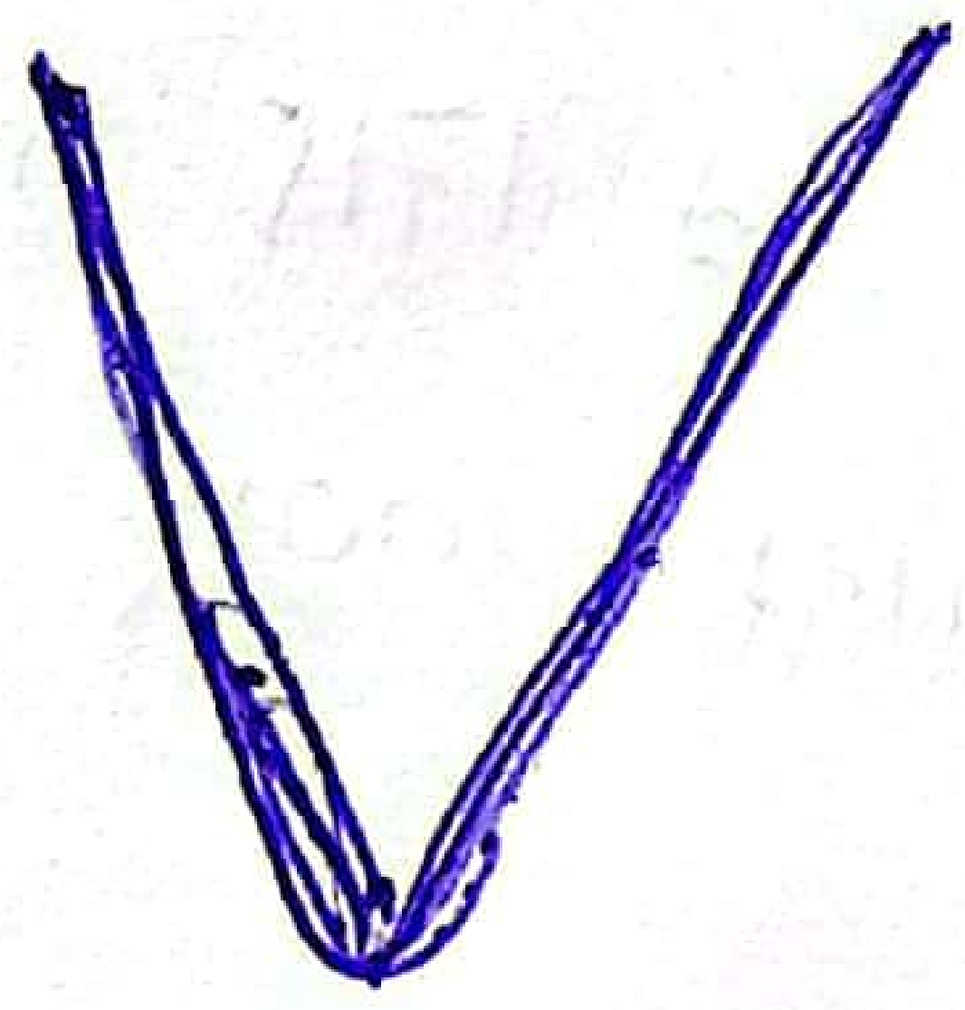
④ H- Bonding :→ stabilized the structure

H-Bonding present in the Alcohols | phenols | carboxylic acid. & Amines (N−H)

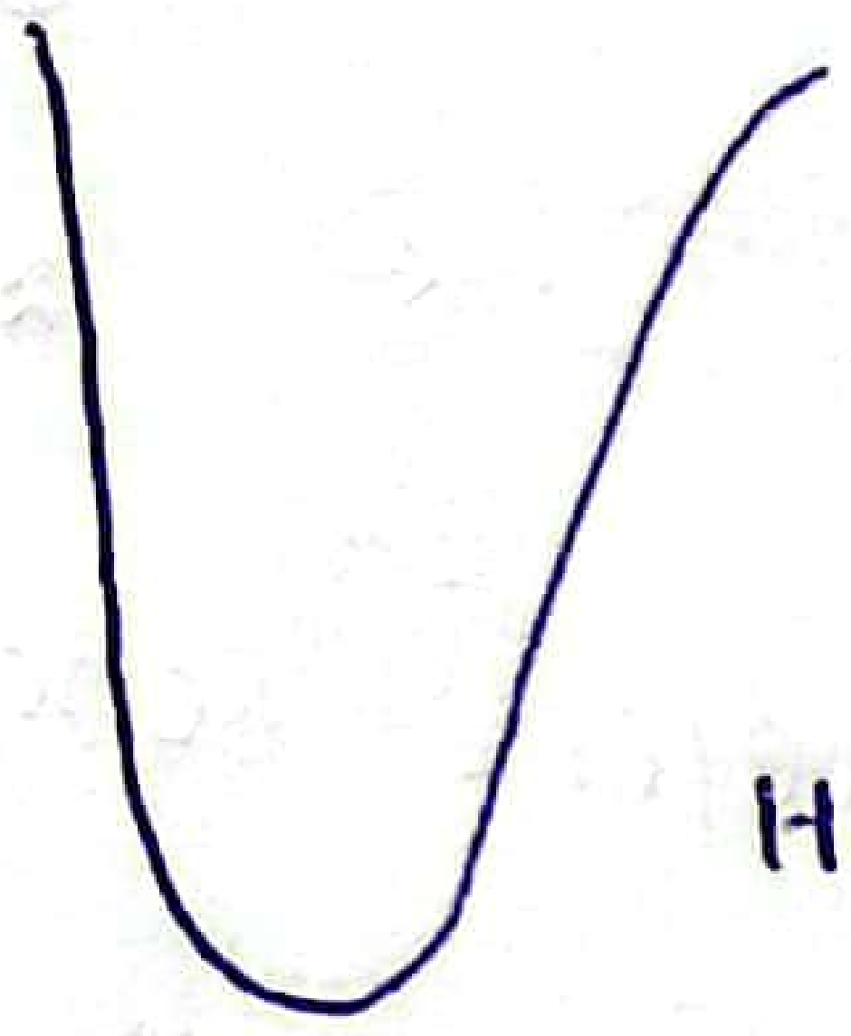
⊛ O−H 3300−3600 cm⁻¹

⊛ O−H
- → H-Bonded → less wavenumber ≈ 3300/3400 cm⁻¹
- → Free from H-bonding → More wavenumber ≈ 3600 cm⁻¹

Sharp peak



Around 3600 cm⁻¹



Broad peak

H-Bonded

~ 3300

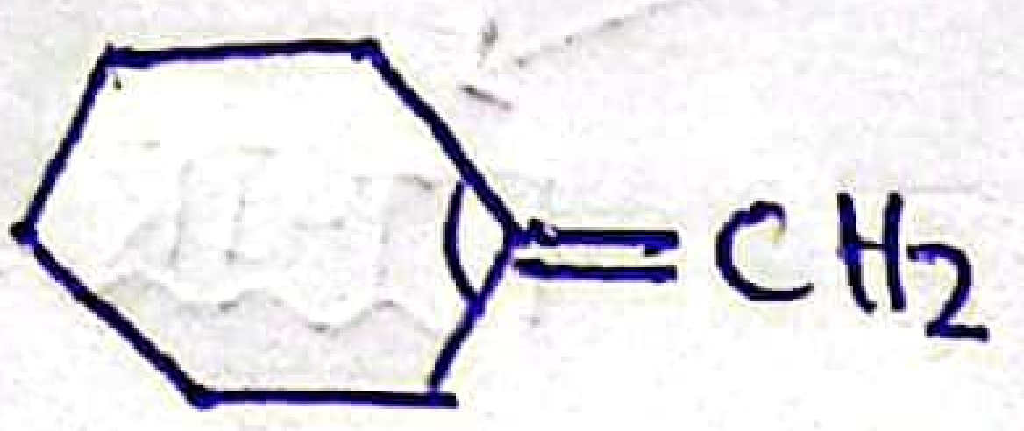
★ N−H → 3300−3400 cm⁻¹

⑤ Angle Strain:

$$\text{internal Angle} \propto \frac{1}{\text{wave-Number}}$$

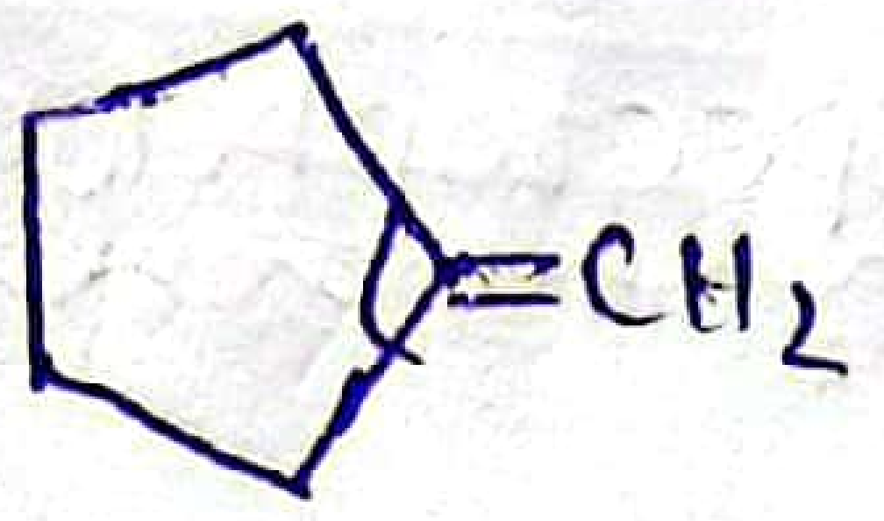
$$\boxed{\text{External Angle} \propto \bar{\nu}\text{-value}}$$

(c=c)



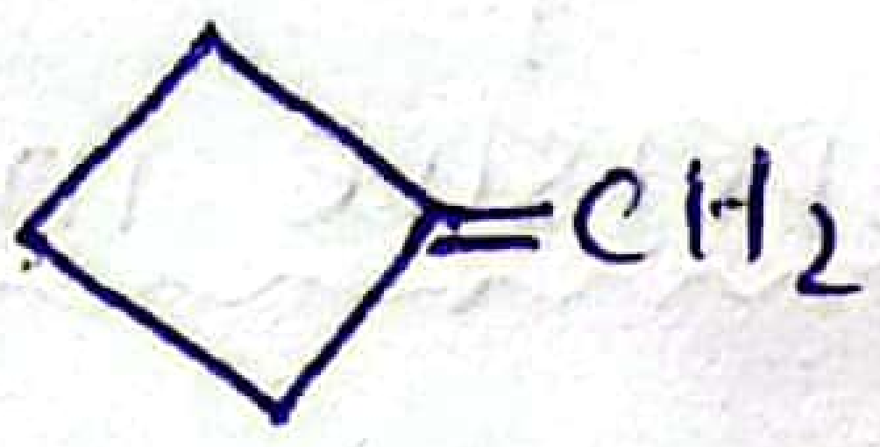
θ = 120°

1650 cm⁻¹



θ = 109°c

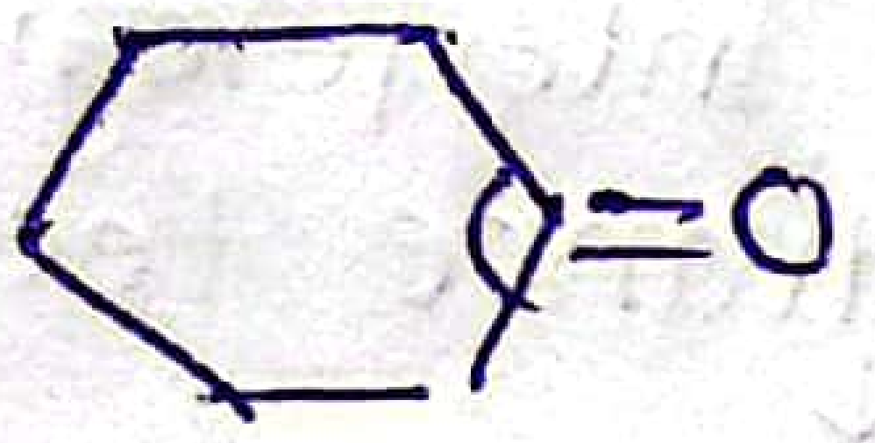
1655 cm⁻¹



θ = 90°

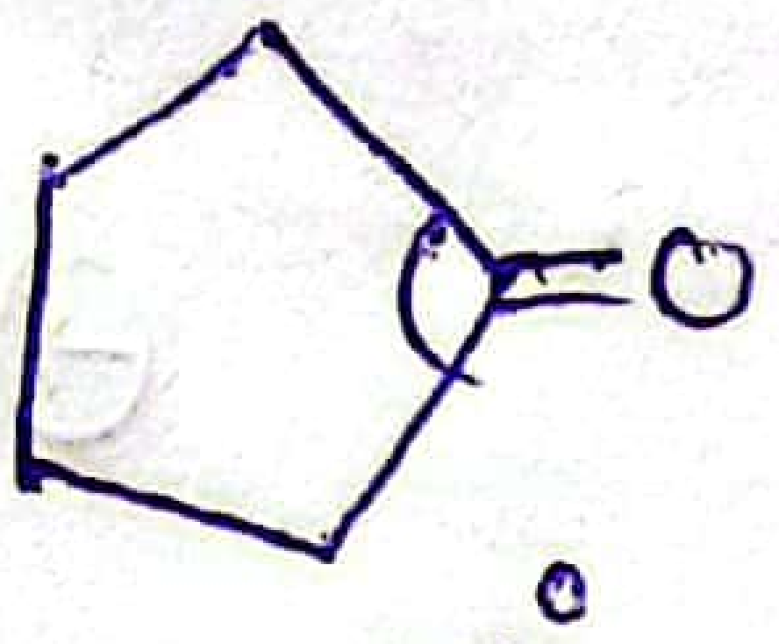
1680 cm⁻¹

(c=o)



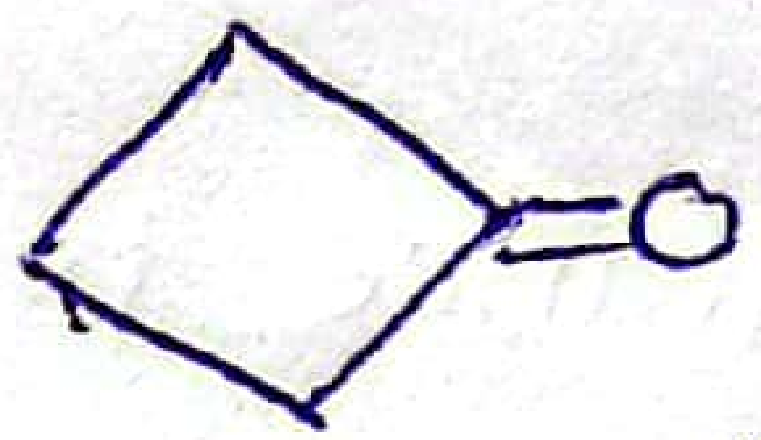
120°

1715 cm⁻¹



109°c

1740 cm⁻¹



θ = 90°

1775 cm⁻¹

⇒ AS internal Bond Angle ~~increas~~ decreases → Thus external Bond Angle increases thus S→ character OF Double Bond increases thus wave No. increases.

↓

Thus Bond strength increases

⑥ Stretching:

∴ Stretching > Bending

∴ Asymmetric > symmetric stretching.

e.g

$$\overleftarrow{O} = C = \overrightarrow{O}$$

1340 cm⁻¹

$$\overrightarrow{O} = C = \overrightarrow{O}$$

2350 cm⁻¹

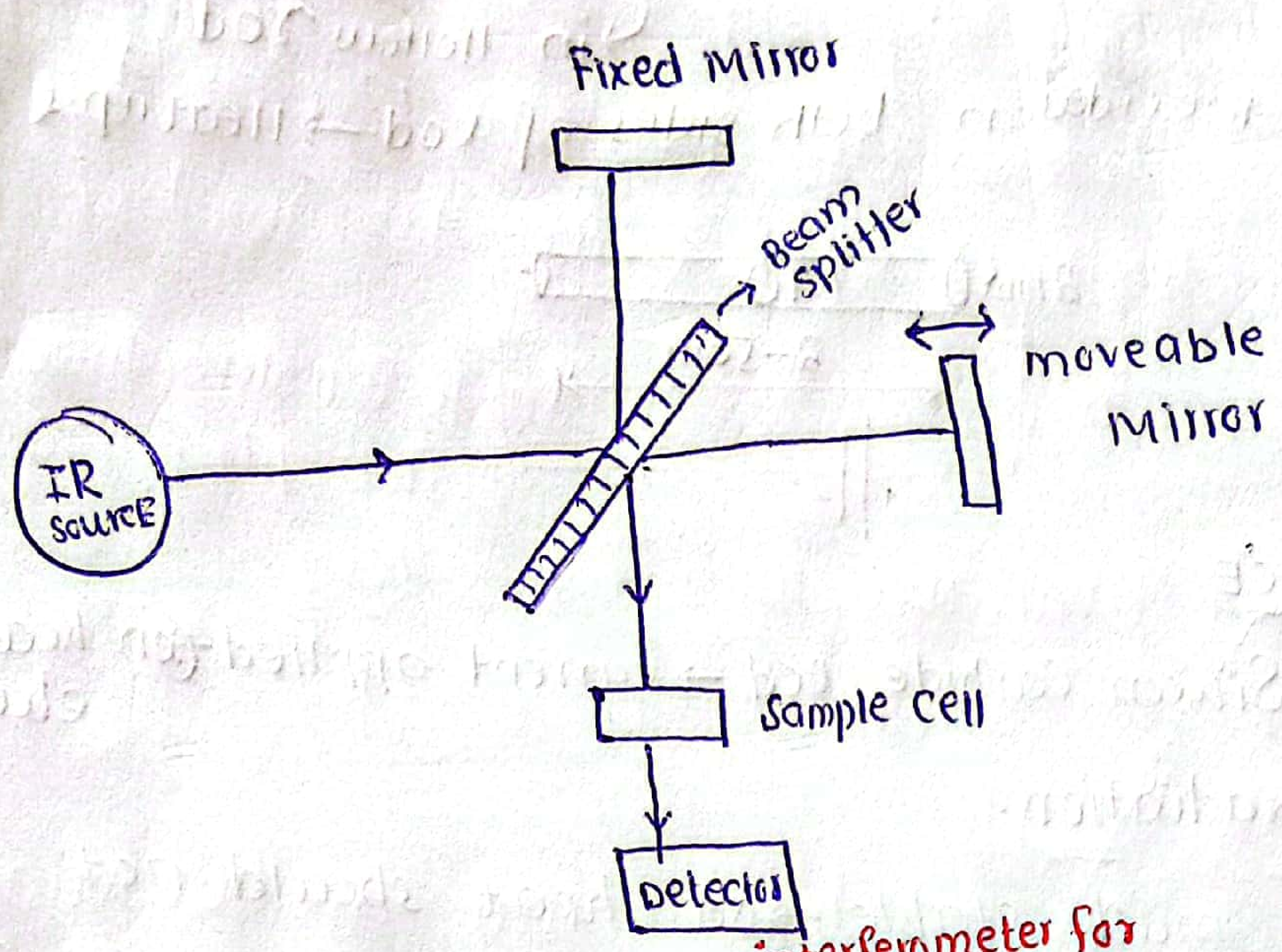
* ——————— *

✓: Instrumentation:

There are two types of IR instruments.

Simple IR spectrophotometer /conventional **Dispersive infrared spectrophotometer**	**FT-IR spectrophotometer**
→ Classical instrument	→ Modern instrument
→ Differaction grating used (to Resolve IR Radiations into individual frequencies) for the Dispersion of λ ↓ Dispersion pattern obtained	→ Interferometer is used. ↓ whole range of IR-used Simultaneously to produce an interferogram → interferance pattern obtained.
→ less Advance technology.	→ more Advance technology ↓ computer & microprocessor Based instrument ↓ mathematical function is used.
	→ spectrum obtained is known as interferogram ↓ time domain But Fousier transformation convert it into frequency domain.
→ lower light throughput	→ Greater throughput → sample sees all λ at a time
→ low Signal-to-noise Ratio	→ Higher Signal to noise Ratio
→ low Resolution	→ High Resolution
→ Generally used in labs	→ used in sophisticated Labs
→ less expensive	→ More expensive
→ Less sensitivity	→ Better sensitivity
→ Less Faster than FTIR	→ Fast → complete a scan 1-2 second.

Sampling Modes techniques in FTIR
- → Reflactance mode (ATR) → No need of sample preparation either solid/liquid.
- → Transmission mode → Need of sample preparation (KBr) disk Required.

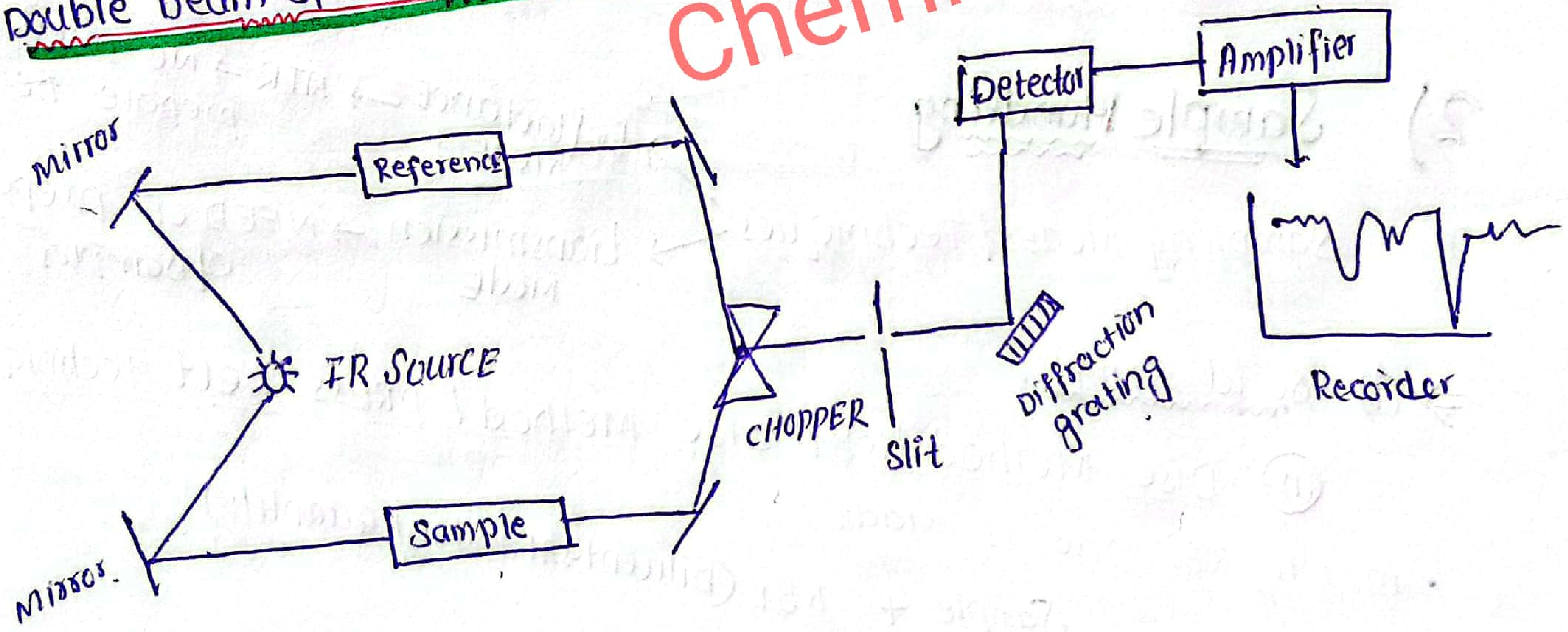


interferometer for (Schematic of (FT-IR Spectrophotometer)

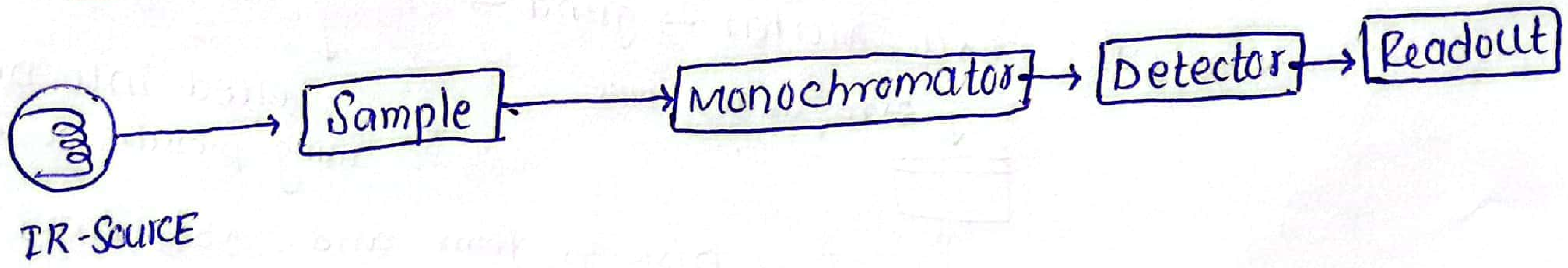
* DISPERSIVE Infrared Spectrophotometer:

↓ Generally this is a Double beam spectrophotometer.

Double beam spectrophotometer



Single beam Spectrophotometer:

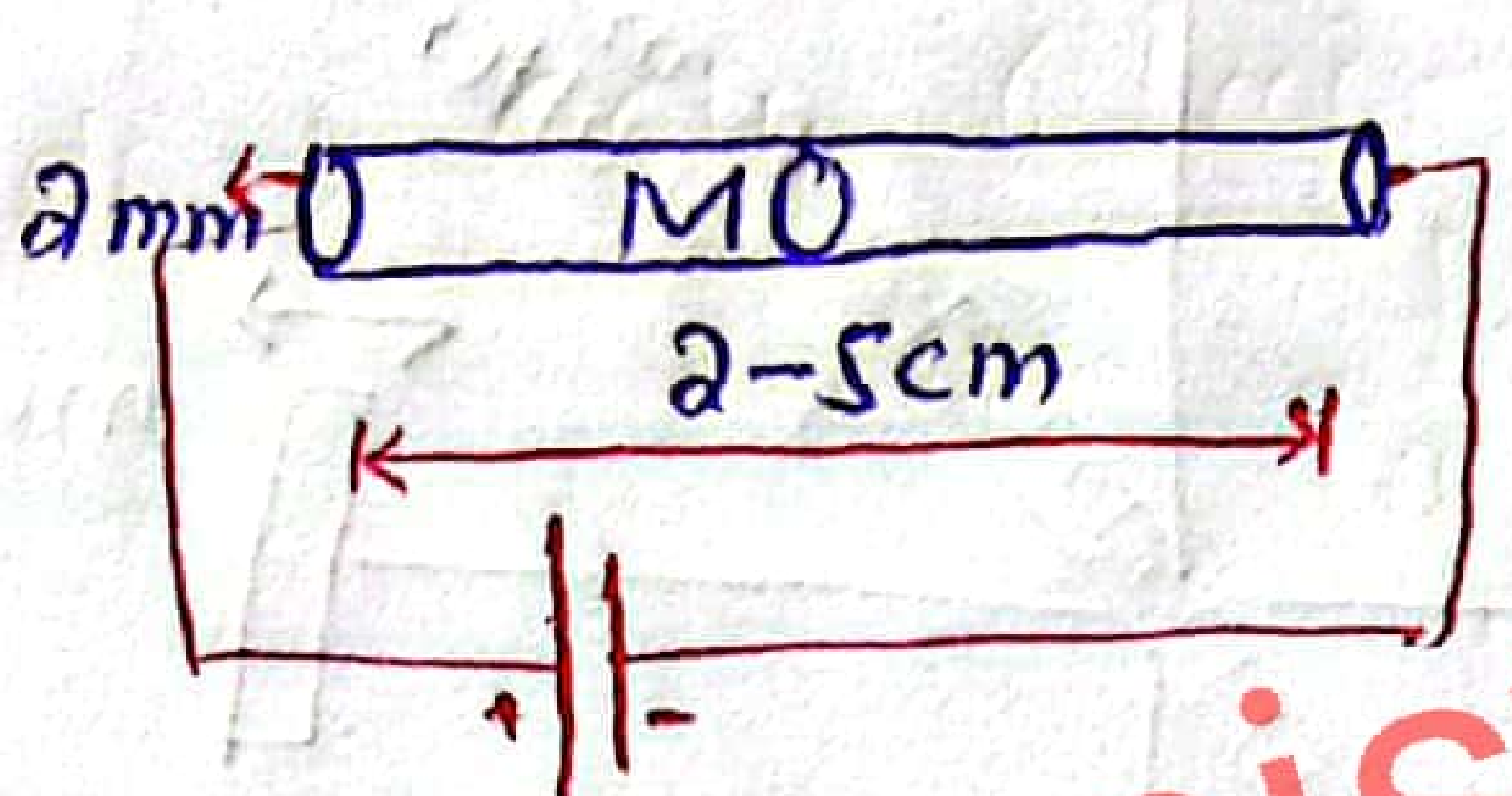


1) IR SOURCE

(i) NErnst Glower source → Metal oxides
e.g oxides oF thorium + Zirconium + yattrium + serium
↳ in Hollow rod

to
e

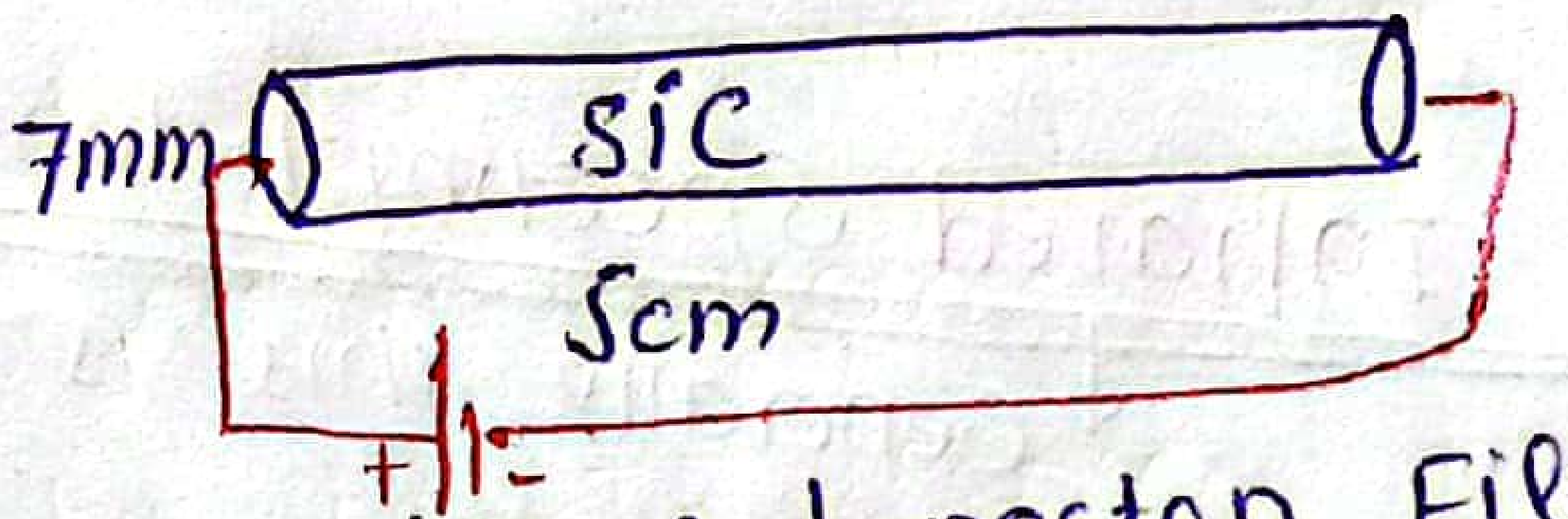
- current is providedon both sides of Rod → Heatup & glows



~~2) Glo~~

(ii) Globar source
↳ Silicon Carbide Rod → current applied (on heating electrically) provide IR Radiation.

★ This is not much stable → so heat should not increase the limit of stability - small voltage is applied As compared to metal oxides.



(iii) Nichrome wire, Rhodium wire & tungston Filament lamp Also used as Radiation source

2) Sample Handling

Sampling modes/Techniques → Reflactance Mode → ATR → NO need to prepare the sample
Sampling modes/Techniques → transmission Mode → NEED OF preparation of Samples

⇒ (i) Solid Sample:

Disc Method / KBr Disc Method / PRESS pelt technique:

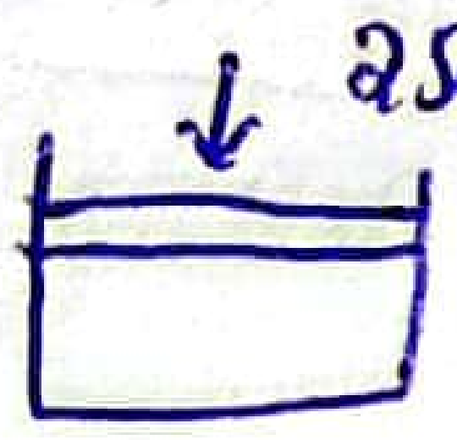
① Disc Method

- in this KBr Disc is made

Sample + KBr (Diluent → Abundant Quantity)
Sample ↓ ~5mg
KBr ↓ ~100mg - 200mg

★ → USE pestle Mortar → grind → powder form
↓
converted into Disc using pressure DEVICE

↓ 25000 pascal pressure



★ when pressure apply → Disk is form and KBr looks like transparent

{ KBr Disk ⇒ diameter 1cm
Thickness 1-2mm

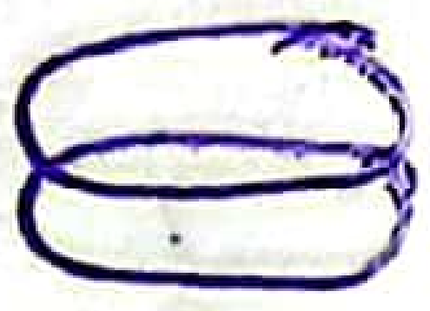
* For making the device you have to use ionic compound e.g KBr/NaCl
↳ b/c (i) IR-transparent
↳ IR inactive
(ii) gets crystal shape → make thin layer

⇒ conditions to make Disc

- High pressure required to make Disc.
- Disc should be clear.
- Sample should be completely dried b/c H_2O is IR active → It will interfere.

(ii) Nujol Mull technique

Sample + Mulling agent ⟶ petridish
↓ 2-5mg
↓ 1-2 drops
↓ *paraffin oil → called Nujol → Hydrocarbons
OR
Thick viscous oil



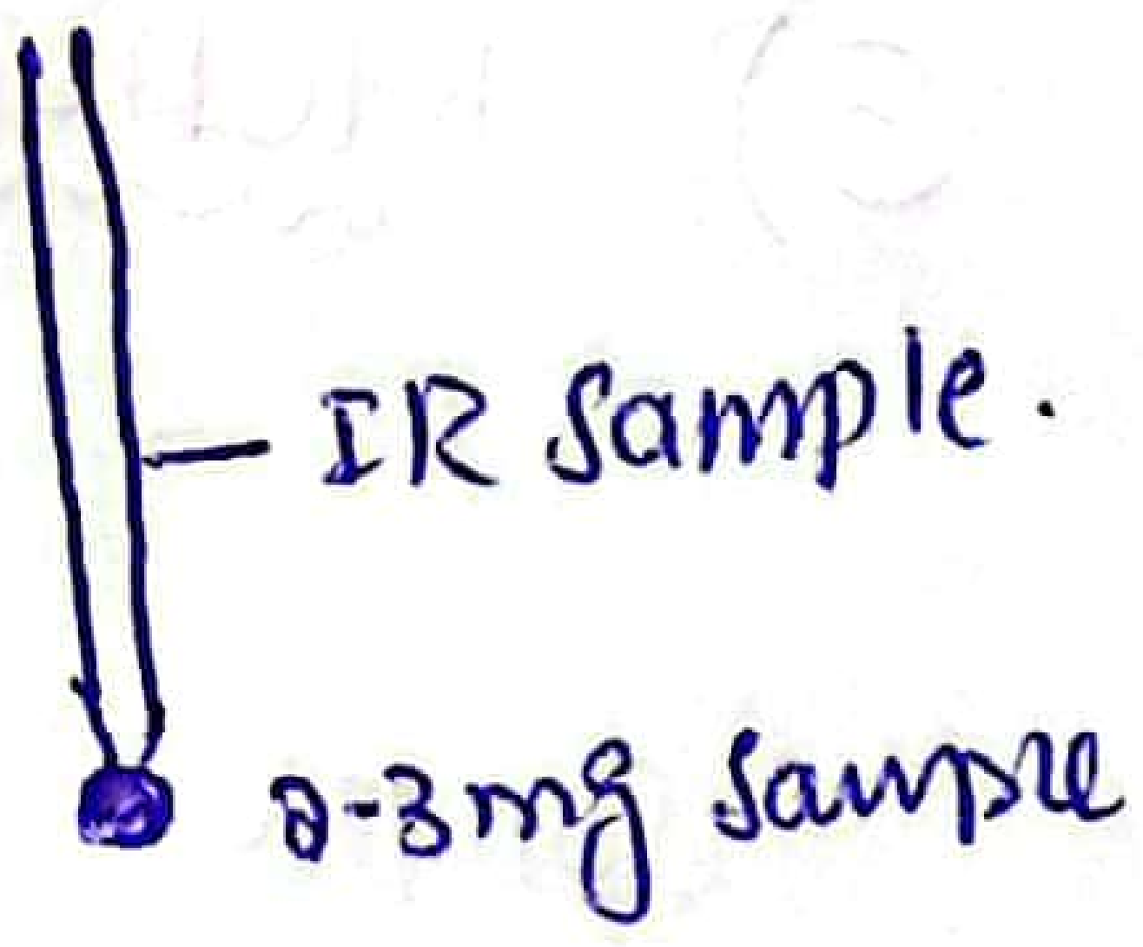
⇒ Make the Homogenous thick paste / Thin film

⇒ These Hydrocarbons show the C-H stretching & Bending peaks and will interfere → but not major interferance.

(iii) Solid State IR → BEST Method.

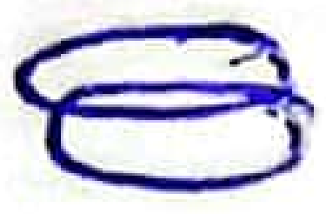
✓ In this NO NEED to make the disc

✓ IR sensor is used → sensor touch the sample



⇒ ii) Liquid Sample preparation:

liquid - liquid → solvent
↓ Sample
↓ petridish is used



Sample examined as Solution in Solvents such as CCl_4, CS_2, $CHCl_3$ etc.

⇒ transparency of Solvent is very important

✓ chloroform less interfere → B/C transparent

* transparency Range ⇒ $CHCl_3$ (4000 – 1500 cm^{-1})
* Carbon Di sulphide ⇒ CS_2 (below 1300 cm^{-1})
* Carbon tetrachloride ⇒ CCl_4 (4000 – 1300 cm^{-1})

transparency Range

↓

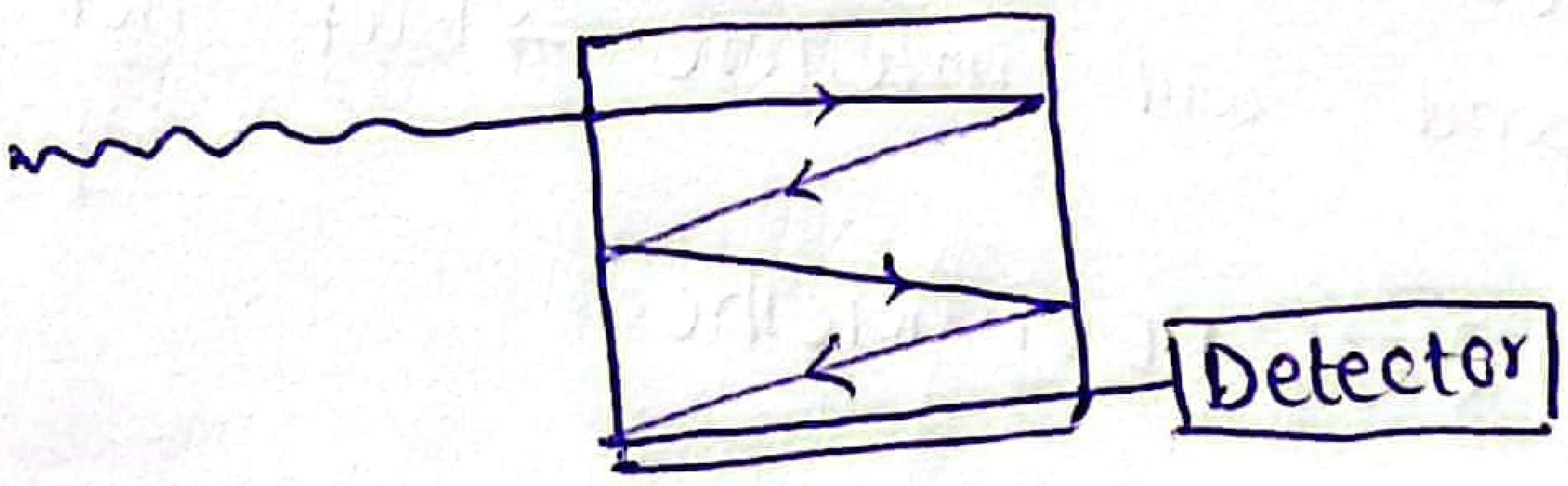
large window Area

Better option

⇒ If CCl_4 not available then use $CHCl_3$

⇒ iii) Gaseous Sample:

A gas sample is introduced into an evacuated gas cell. Gas cell available from few cm to some meters. But problem is that Sampling Area will not accomodate cells longer than 10cm. So Gaseous Sample is Analyzed by the IR Sensor by Multiple internal Reflection due to increase of path length.



⇒ IR probe is used

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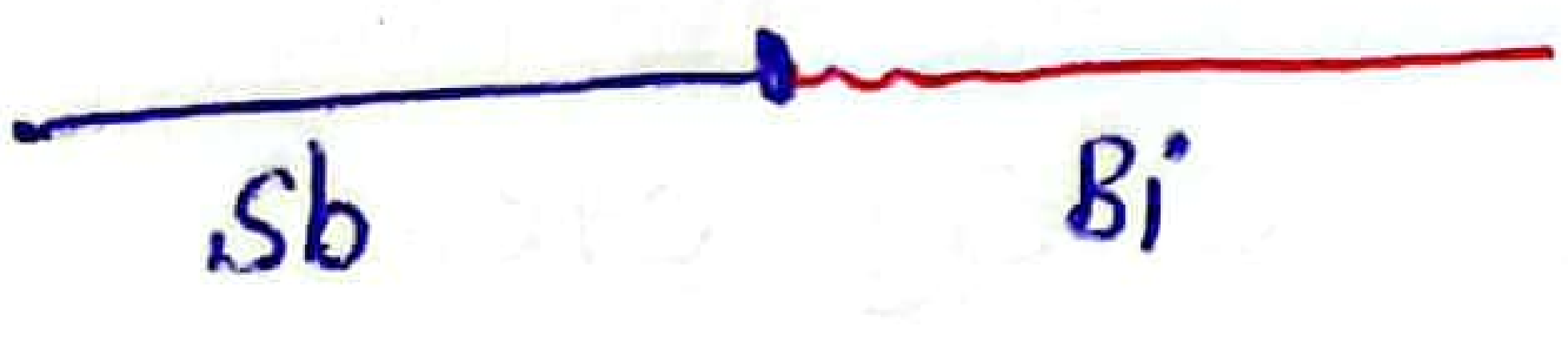
3) Monochromator:

In IR monochromator is kept After the sample to stop the stray & scattered IR Radiations.

4) Detector

Thermal Detector is used in IR → works on the principle of Thermocouple.

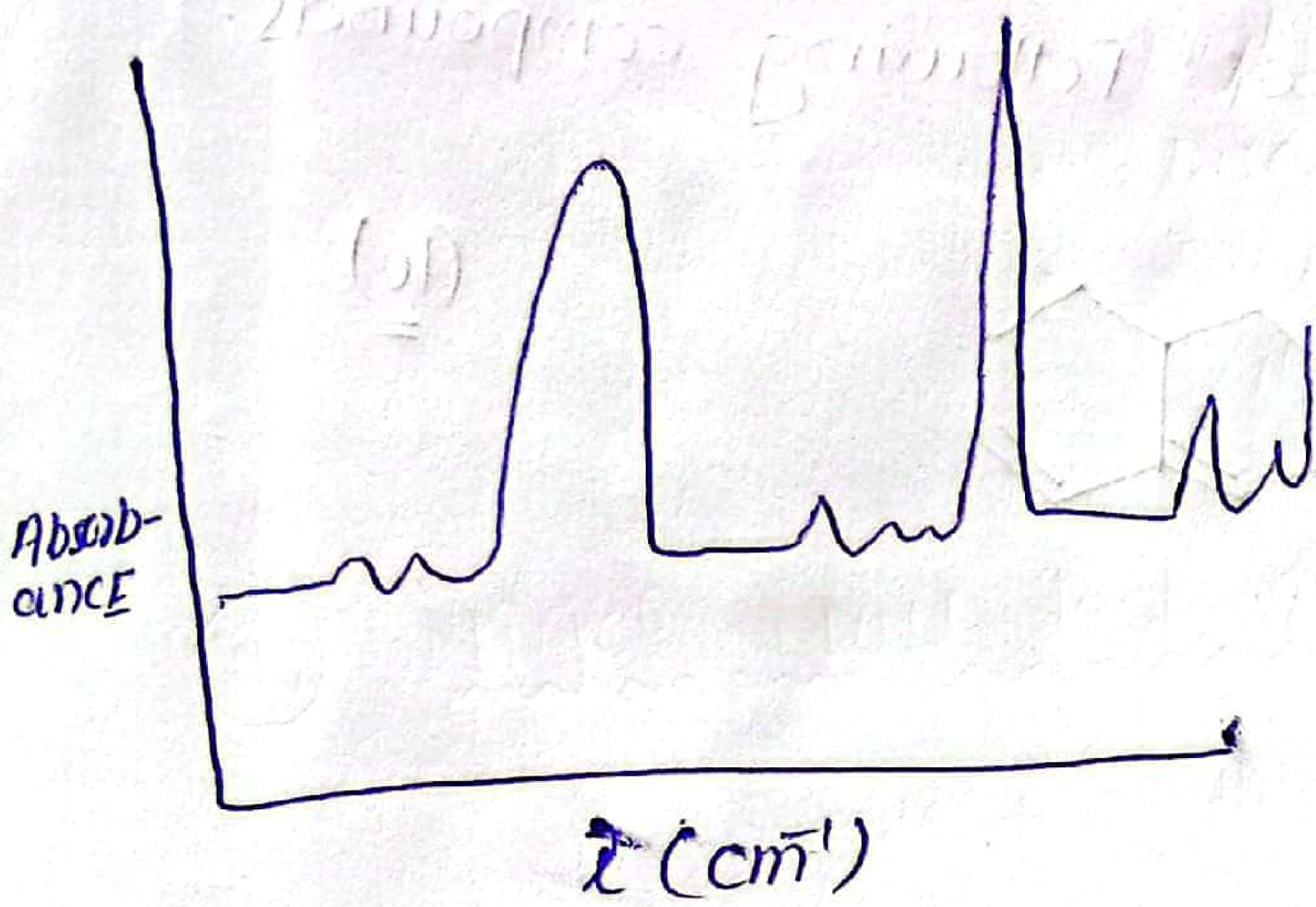


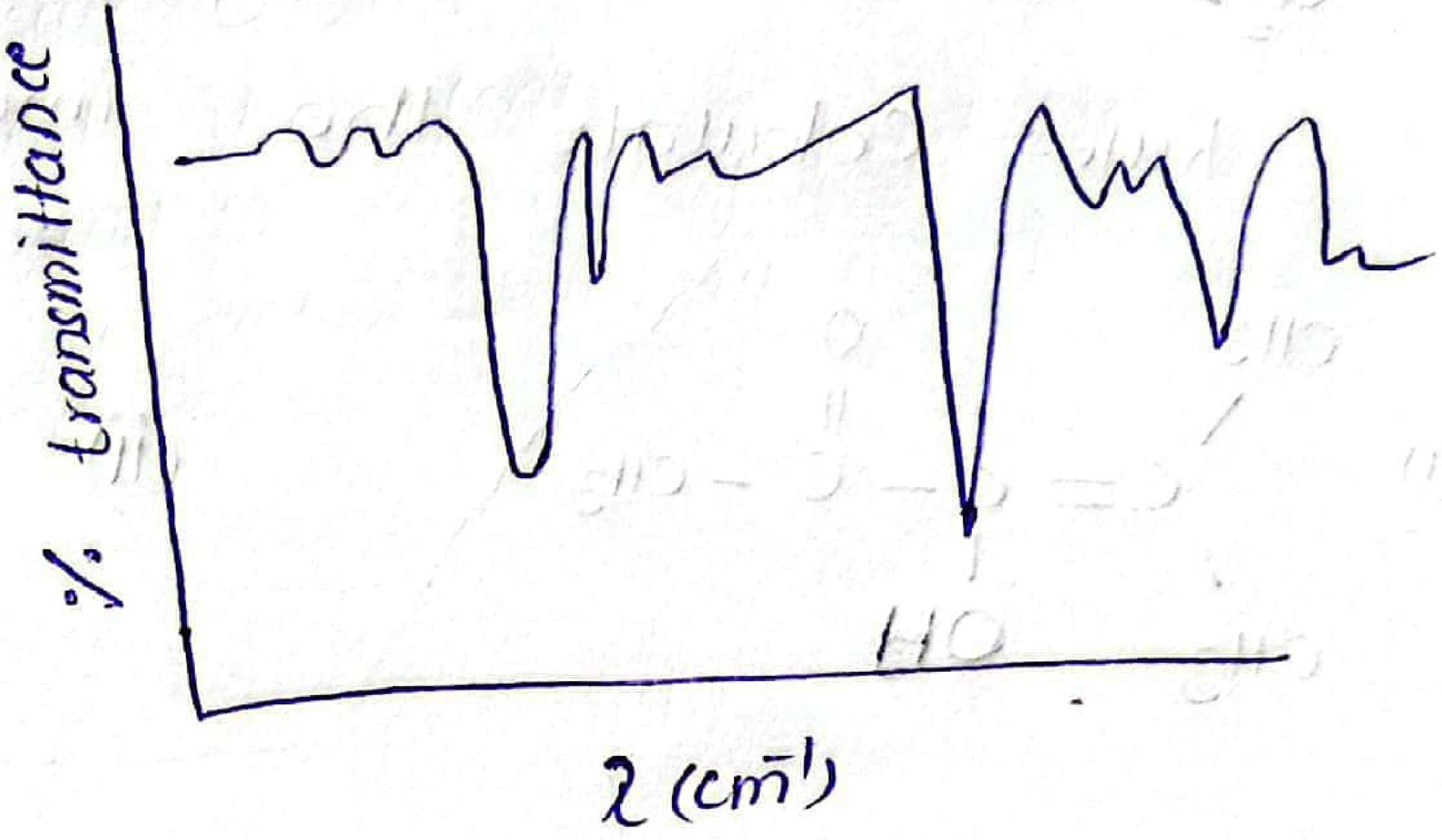
two wires of dissimilar Metals are joined. when diff. of T is ~~caused~~ created at the junction current is flow

~~Thermocouple~~ Due to Flow of current → Heat energy is produced. Thermocouple convert this heat energy into electrical energy.

* Current produced ∝ Intensity of IR-Rad falling on Detector.

5) Read out device:





(INTERPRETATION OF IR-SPECTRA)

Mid-IR is characteristic for each functional group. **4000 – 400 cm^{-1}**

or

4000 – 667 cm^{-1}

We divide it into 4-regions.

(1) H-bond region / Lighter region **(4000 - 2200 cm^{-1})**
(2) Triple-bond region **(2250 – 1850/2000 cm^{-1})**
(3) Double-bond region **(2000/1500 cm^{-1})**
(4) Finger-print region / Heavier region **(<1500 cm^{-1}**

(1) H-Bond region:-

Peaks of -OH, C–H, N–H, S–H are obtained **D–H** (protium)

(2) Triple bond region:-

$C\equiv C$, $C\equiv N$ (Nitrile) peaks.

$C=C=C$ (Ketenes) **two 2ble bond = 3rple bond.**

(3) Double b

$C=C$, $C=O$

(4) Finger

C–O, N–O, C–N, C–X, C–F, C–Cl, C–Br, C – transition metal.

$C-H$ = 3300 – 2850 cm^{-1}
$O-H$ = 3200 – 3800 cm^{-1}
$N-H$ = 3200 – 3400 cm^{-1}

→ Less characteristic region. Bending vibrations are observed here (<1500 cm^{-1})
→ Very difficult to observe.

*→ **Stretching vibrations** are characteristic for the identification of compound.
*→ IR – does not give complete structure of compound, but expected (family)

* C–H peaks :-

Stretching + Bending both are included in peaks.

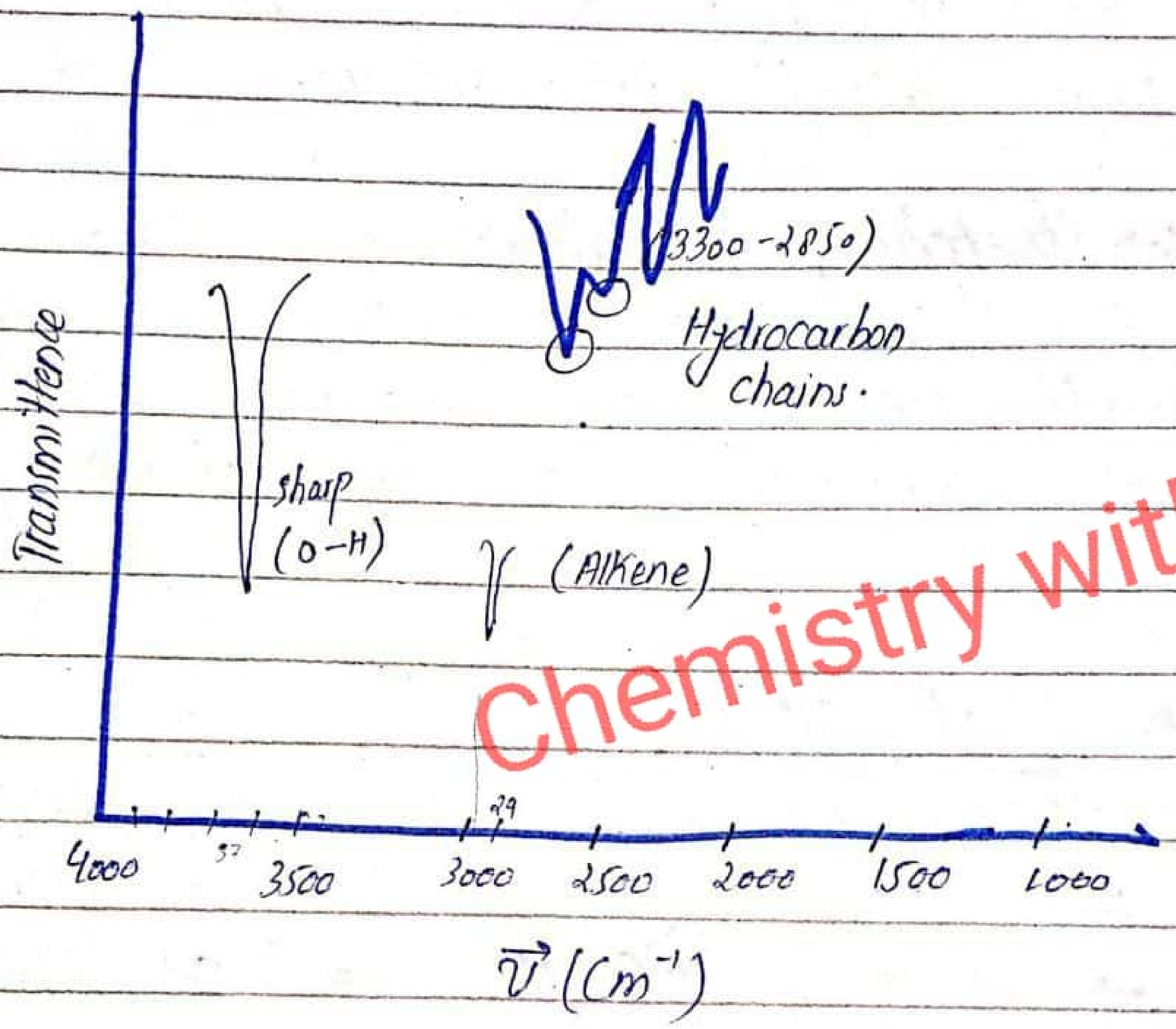
(C–H– stretching)

→ Alkanes, $-\overset{|}{\underset{|}{C}}-H$ = 3000 – 2900 cm^{-1}
→ Alkene $C=C-H$ = 3100 – 3000 cm^{-1}
→ Alkyne $C\equiv C-H$ = ~ 3300 cm^{-1} very near
→ Aldehyde $O=C-H$ = Two peaks ~2850 cm^{-1}
2750 cm^{-1}

* **Range** = 3300 – 2850 cm^{-1}

Alkyne ——— O-H
↓
Addition peak (3300-2850 cm⁻¹) CH_3-C-CH_3

Spectra :-



*** O-H peaks :-**
→ Hydrogen bonded (3200-3400) (↑ high peak) Broad peak.
→ Free O-H (Sharp peak) (3600-3700)

*** Range :** (3200-3800 cm⁻¹)

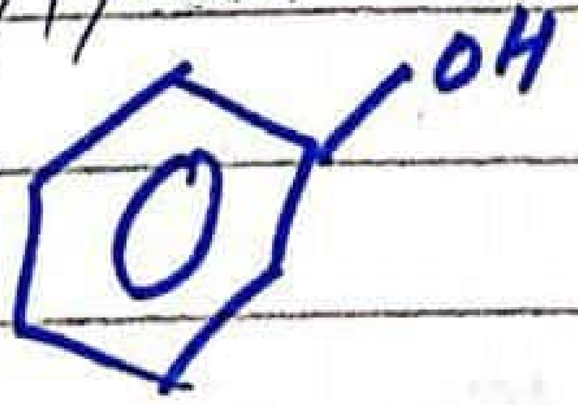
(Alcohol, Phenols / carboxylic acids) are indicated not confirmed.

Not characteristic

characteristic

① **Alcohols** $CH_3CH_2 - OH$

② **Phenol** : Three/4 peaks are obtained.



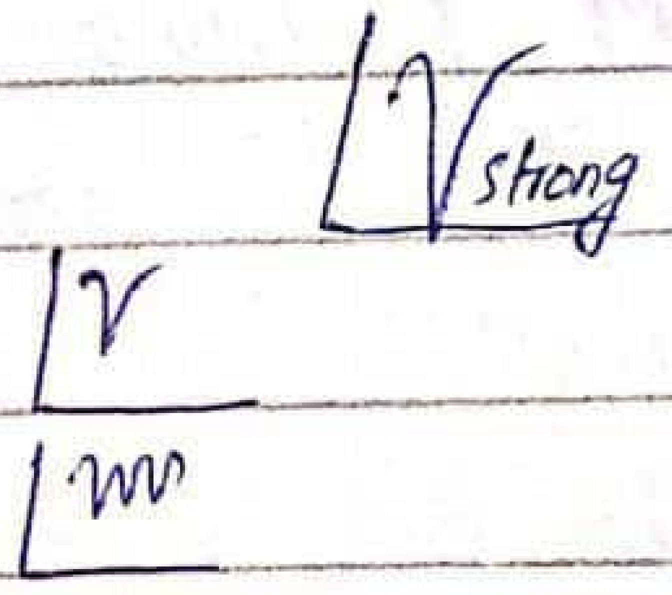
(1) O–H = peak.
(2) C–C = peak
(3) C–O = peak.
(4) C=C = peak

$C-O = 1300-1000cm^{-1}$
$C-C = 1200\ cm^{-1}$
$C=C = 1650$ (S)

In case of **Aromatic / Benzene** two peaks are obtained.
(1) ~1500 (2) ~1600

Peaks

(S) Strong peak
(m) Mediocre
(w) Weak.



(Intensity)

$-\overset{O}{\overset{\|}{C}}-$ is intense peak obtained around

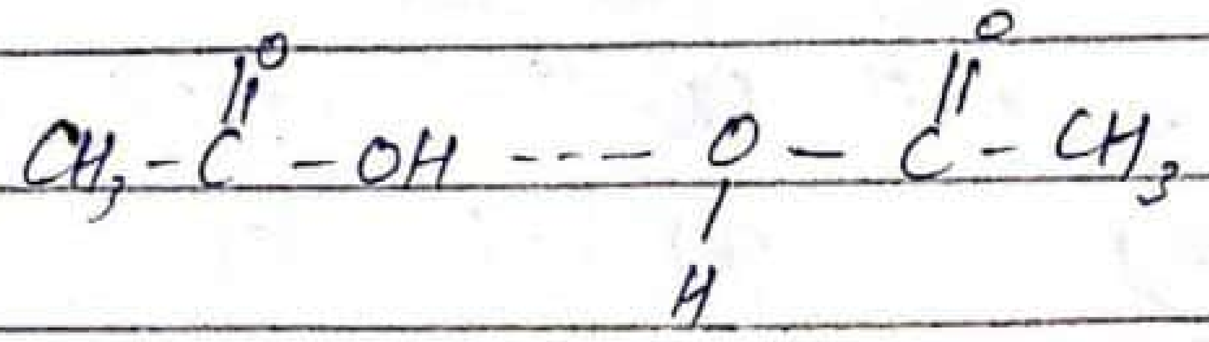
③ **Carboxylic acid** :- $-\overset{O}{\overset{\|}{C}}-OH$

O–H peak
$\overset{O}{\overset{\|}{C}}-H$ peak
C–O

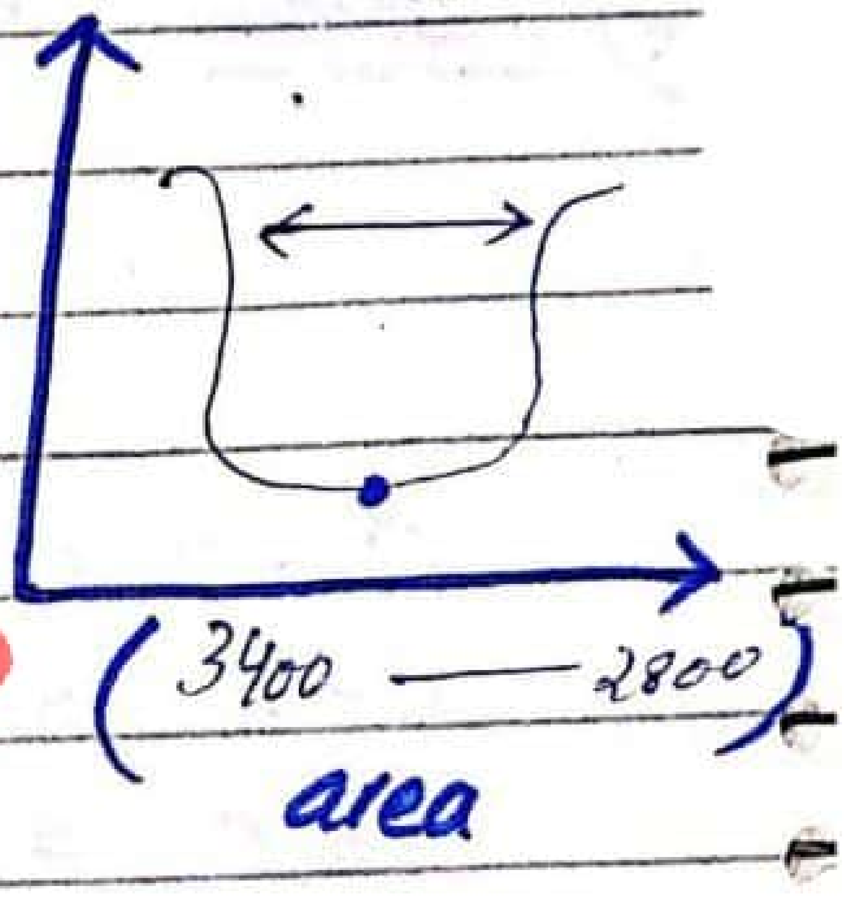
{Additional Peaks} differenciate b/w functional groups.

→ Carboxylic acid show (hydrogen bonding).

→ **Much Broader peak** is obtained.



$CH_3-C(=O)-OH\cdots O(H)-C(=O)-CH_3$



→ **Area = 3400 - 2800 cm^{-1}**

→

*** N-H peaks :-** ($3200 - 3400\ cm^{-1}$)

differentiat N-H —?— OH —?— C≡C

(1) Amines (Primary + Sec + Tertiary)

P = CH_3NH_2 = Two sharp peaks. **S =** 1 peak. N

T = No peak

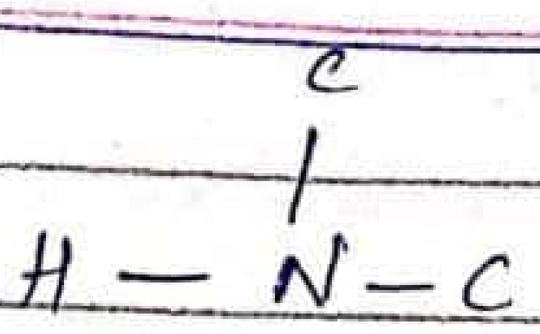
(2) Amides.

→ In (N-H) it is sharp.

→ In (O-H) region it is broad as it is sharp in ($3600\ cm^{-1}$)

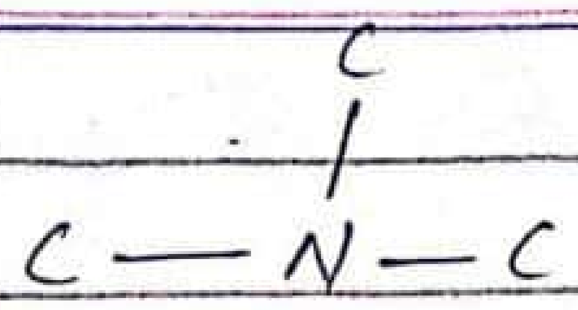
(3) C-N ($1000 - 1350 cm^{-1}$)

NH, OH, [illegible], C-H



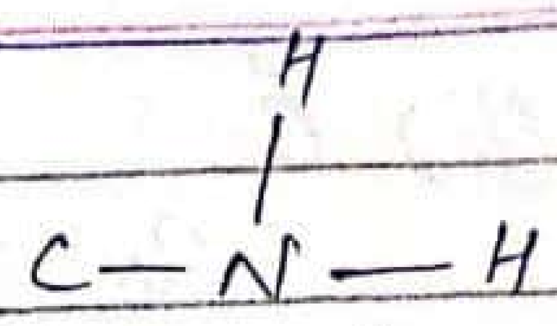
$H-\overset{\overset{C}{|}}{N}-C$

1 peak



$C-\overset{\overset{C}{|}}{N}-C$

No peak



$C-\overset{\overset{H}{|}}{N}-H$

2-peak

Amine = N-H = 3300-3400

Alkyne = $C\equiv C-H$ = 3300

How will you identify from them?

(1) There will be no $C\equiv N$ peak

Ans

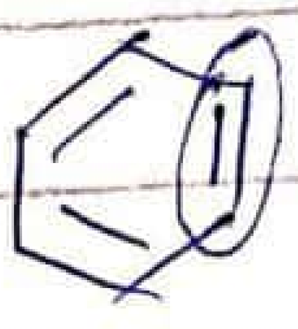
* Alkyne = $C\equiv C-H$ (2150) cm^{-1}

* $C\equiv N$ has more intensity than $C\equiv C$

* **IR- Co-relation Chart:-** Study

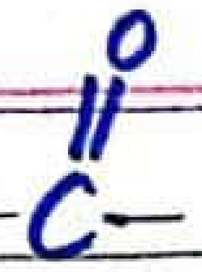
* **C=C peaks**

~ (1650 cm^{-1})

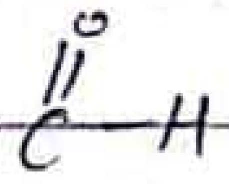


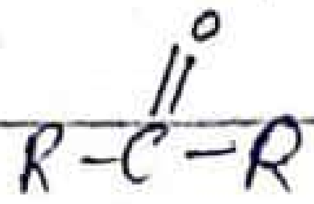
conjugation is involved

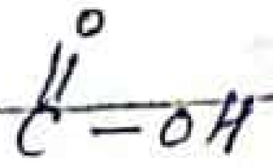
$\bar{\nu}$ will ↓ with ↑ in stretching so, $\bar{\nu}$ will be lower than 1650 cm^{-1}

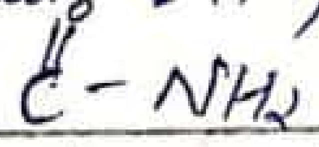
(ii) 
$-\overset{\overset{O}{\|}}{C}-$ (1600 - 1800 cm^{-1})

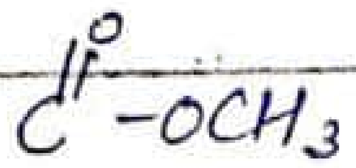
Carbonyls

↳ Aldehydes ~1725 
$\overset{\overset{O}{\|}}{C}-H$

Ketone ~1715 
$R-\overset{\overset{O}{\|}}{C}-R$

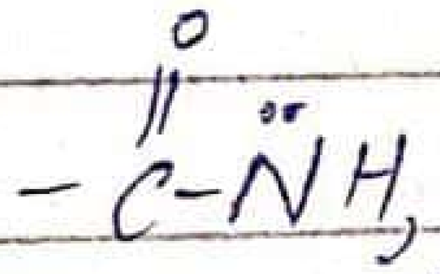
C.acids. ~1710/1700 
$\overset{\overset{O}{\|}}{C}-OH$

Amides ~1690
(only compounds whose peak ↓ 1700) 
$\overset{\overset{O}{\|}}{C}-NH_2$

Esters ~1735 
$\overset{\overset{O}{\|}}{C}-OCH_3$

Anhydrid. ~1765

(Acid-halides) ~1800

-: **Amides** 
$-\overset{\overset{O}{\|}}{C}-\ddot{N}H_2$ has lone pair, increases much stretching so $\bar{\nu}$ ↓↓↓

Acid halide	**Anhydride**	**Esters**	**Ald.**	**Ketones.**	**C.acid**	**Am**
1800	1765	1735	1725	1715	1710	169

Aldehydes / Ketones differenciate. ??

C-H (str.) is observed and two peaks will obtain

How

if CH_3 + CH_2 than 3 peaks.
(2900 - 3000) cm^{-1}

(Carboxylic + Amides)
↓ O-H will be broade.

✓

$C-F = 1100 - 1000\ cm^{-1}$
$C-Cl = 750\ cm^{-1}$ (+,- 30)
$C-Br = 550/600\ cm^{-1}$

IR Correlation Chart:

(4000–400/667 cm^{-1})

Bond Regions	Range	Constituents
H-Bond / lighter Region	4000–2200 cm^{-1}	–OH –C–H N–H S–H C–~~D~~H (Protium)
Triple Bond Region	2250–1850/ 2000 cm^{-1}	C≡C (2150 cm^{-1}) C≡N (Nitrile) C=C=C (Ketene)
Double Bond Region	2000/1500 cm^{-1}	C=C (1650 cm^{-1}) C=O 1600-1800
Finger Print Region	< 1500 cm^{-1}	C–O , C–Br N–O , C–Cl C–N , C–F C–X , C–t.metal

(C-H Peaks) (C-H stretching)

(3300–2850) cm^{-1}

Names	f. Group	Range
Alkanes	–C–H	3000–2900 cm^{-1}
Alkenes	C=C–H	3100–3000 cm^{-1}
Alkynes	C≡C–H	~ 3300 cm^{-1}
Aldehydes	O=C–H	① 2850 cm^{-1}
		② 2750 cm^{-1}

C-H peaks = 3300–2850 cm^{-1}
O-H peaks = 3200–3800 cm^{-1}
N-H peaks = 3200–3400 cm^{-1}
C.acid peaks = 3400–2800 cm^{-1}
Carbonyl peaks = 1600–1800 cm^{-1}

(O-H Peaks)

(3200–3800) cm^{-1}

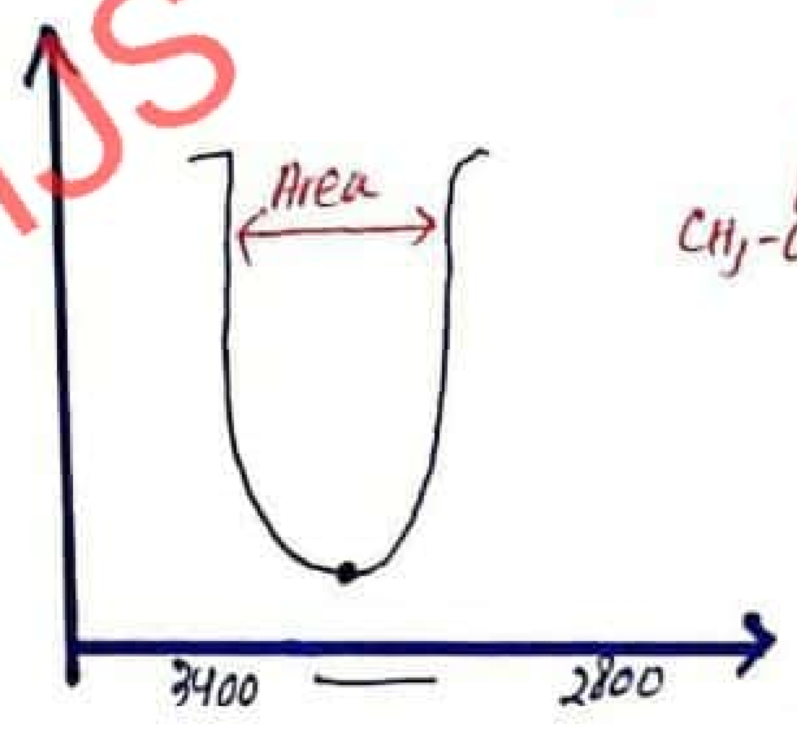
Names	Constituents	Peaks Ranges
O-H Peaks	Bonded Hydrogen	(3200–3400) cm^{-1} (Broad peak)
	Free Hydrogen	(3600–3700) cm^{-1} (Sharp-peak)
* Alcohols (1) C–O ⇒ 1300–1000 cm^{-1} (2) C–C ⇒ ≃1200 cm^{-1}	(R–OH)	(3) OH (3200–3400) cm^{-1}
Phenols	O–H	(3200–3400) cm^{-1}
	C–C C=C	(1200 cm^{-1}) (1650 cm^{-1})
	C–O	(1300–1000 cm^{-1})
	Aromatic ring	~ 1500 cm^{-1}
		~ 1600 cm^{-1}

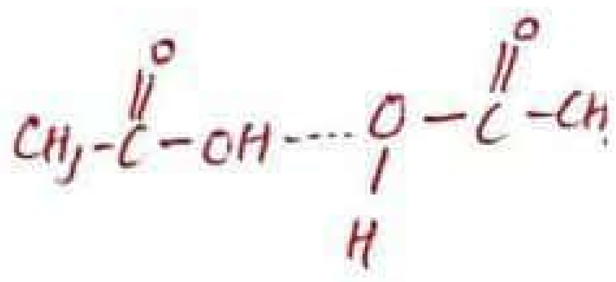
(Carboxylic Acid) :-

(3400–2800) cm^{-1}

Names	"	Ranges
O–H	Broad Peak	(3200–3400) cm^{-1} wide
$\overset{O}{\overset{\|}{C}}-H$	sharp peak	(1700–1800) cm^{-1}
C–O		(1300–1000) cm^{-1}

Due to "Hydrogen-Bonding" much broader peak is observed Covering area (3400–28





$CH_3-\overset{O}{\overset{\|}{C}}-OH\cdots\underset{H}{\underset{|}{O}}-\overset{O}{\overset{\|}{C}}-CH$

(N-H Peaks)

$(3200-3400)\,cm^{-1}$

Names	"	Peaks
Amines $R-N\begin{smallmatrix}H\\R\end{smallmatrix}$	Primary = Two sharp peaks	$(3300-3400)\,cm^{-1}$
	Secondary = 1 peak	
	Tertiary = 0 peaks	
* Amides $R-\overset{O}{\overset{\|}{C}}-NH_2$	N-H = Sharp $C=O$ = 1600-1800 cm^{-1}	$(1690)\,cm^{-1}$
C-N	$H-\overset{C}{\overset{\|}{N}}-C$ (1peak)	$(1000-1350)\,cm^{-1}$
	$C-\overset{C}{\overset{\|}{N}}-C$ (0 peak)	
	$C-N\begin{smallmatrix}H\\H\end{smallmatrix}$ (2peak)	

(Carbonyl-Peaks):

$(1600-1800)\,cm^{-1}$

Names	"	Peaks
Acid Halide	$R-\overset{O}{\overset{\|}{C}}-X$	$1800\,cm^{-1}$
Anhydride	$-\overset{O}{\overset{\|}{C}}-O-\overset{O}{\overset{\|}{C}}-$	$1765\,cm^{-1}$
Esters	$-\overset{O}{\overset{\|}{C}}-OR$	$1735\,cm^{-1}$
Aldehydes	$-\overset{O}{\overset{\|}{C}}-H$	$1725\,cm^{-1}$
Ketones	$R-\overset{O}{\overset{\|}{C}}-R$	$1715\,cm^{-1}$
C. Acids	$R-\overset{O}{\overset{\|}{C}}-OH$	$1710\,cm^{-1}$
Amides.	$-\overset{O}{\overset{\|}{C}}-NH_2$	$1690\,cm^{-1}$

$C-N$ = $1000-13500\,cm^{-1}$

$C-O$ = $1000-1300\,cm^{-1}$

$NO_2 = \begin{cases} \rightarrow 1350\,cm^{-1} \\ \rightarrow 1550\,cm^{-1} \end{cases}$

Aromatic = $\overset{①}{1500} + \overset{②}{1600}\,cm^{-1}$

$\underset{O}{\underset{\|}{C}}$ = (1600-1800) 1 peak

F. Groups	Peaks
C-F	$1100-1600\,cm^{-1}$
C-Cl	$750\,cm^{-1}$
C-Br	$550/600\,cm^{-1}$

Mainly differenciated due to Carbonyls.

---

* How to differenciate b/w **NH, OH & C-H**

* N-H = sharp peak
* O-H = Broad in this region
* C-H = $3000-2900\,cm^{-1}$

---

* How to differenciate b/w **C≡C-H N-H**
(Alkyne) (Ammine)

as they have:

N-H = $3300-3400\,cm^{-1}$

C≡C-H = $3300\,cm^{-1}$

→ since there will be No C≡N peaks in alkynes.

---

* How to differ. **Alkynes & Nitriles**

Alkyne = C≡C-H = $2150\,cm^{-1}$

Nitrile = C≡N- = $2250\,cm^{-1}$

---

* How to differ **Aldehyde & Ketone?**

Aldehyde = 2 peaks will be observed.
$(2900 + 3000)\,cm^{-1}$

---

* How to differ **C.acid & Amide?**

(O-H) will be broader in Carboxylic acid.

*In amide two peaks of -NH

Applications:

UV = Quantification ↑ + ↓ Quality
IR = ↑ Qualitative + ↓ Quantitative.

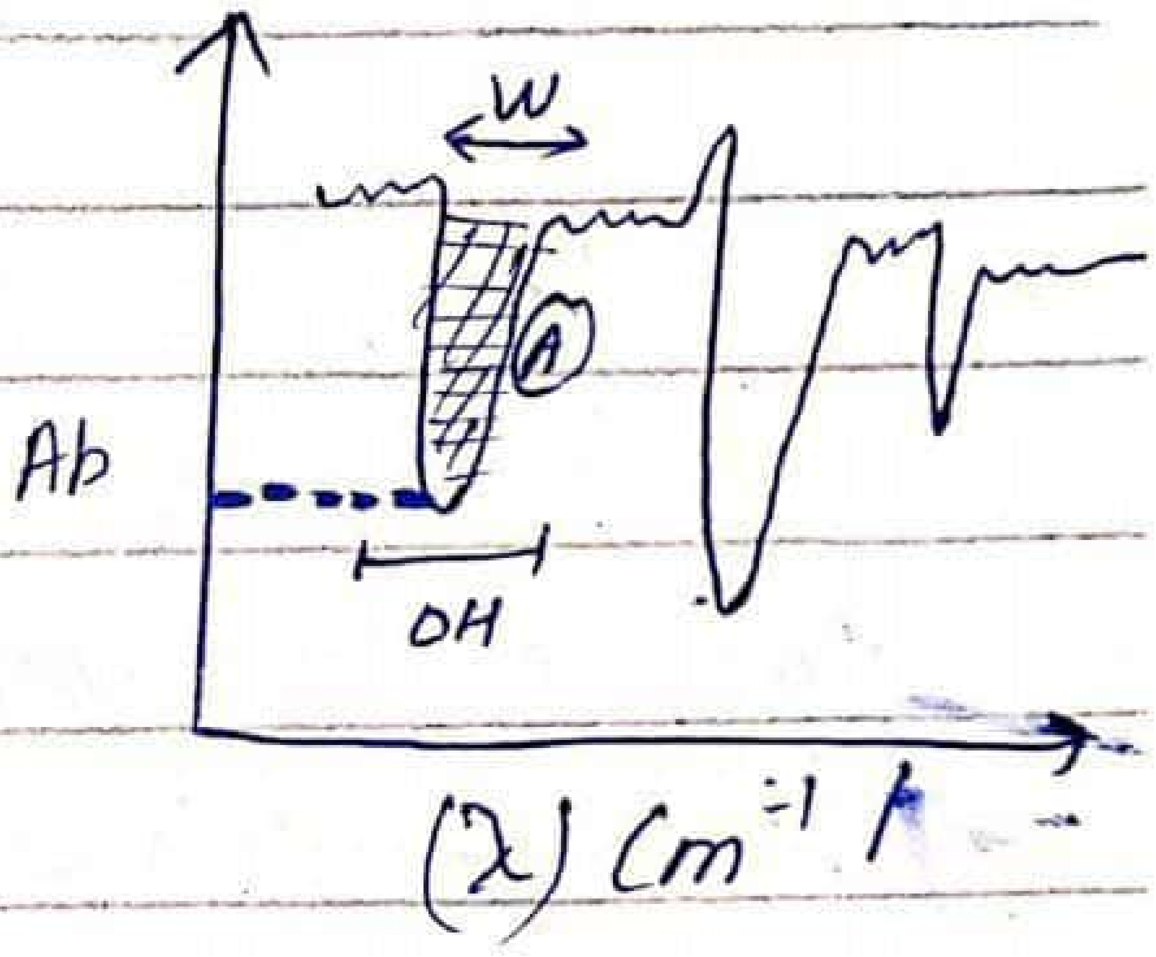
(1) Structure elucidiation:-

Compared with standard spectra.

(2) Identification of functional groups:

Qualitative Study

By assigning the peaks. Which one is absent.



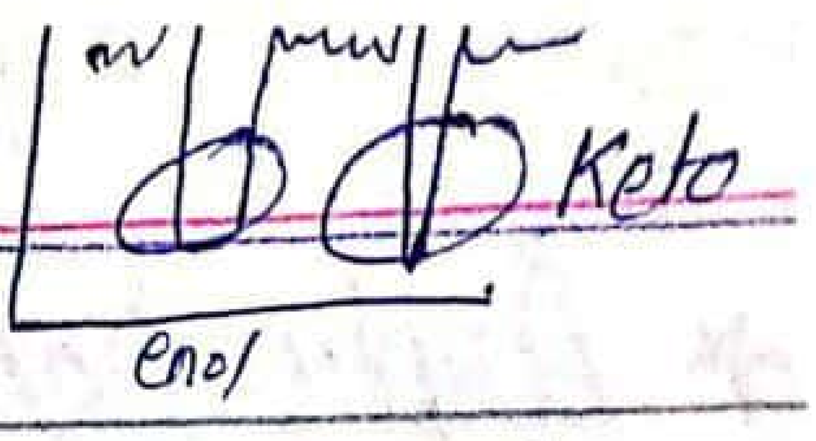
(3) Quantitative Study:-

Let.

Moisture determination.

Due to moisture **-OH** peaks are obtained. which is broader. The area & width is taken and its quantification is done.

But this is not authentic.

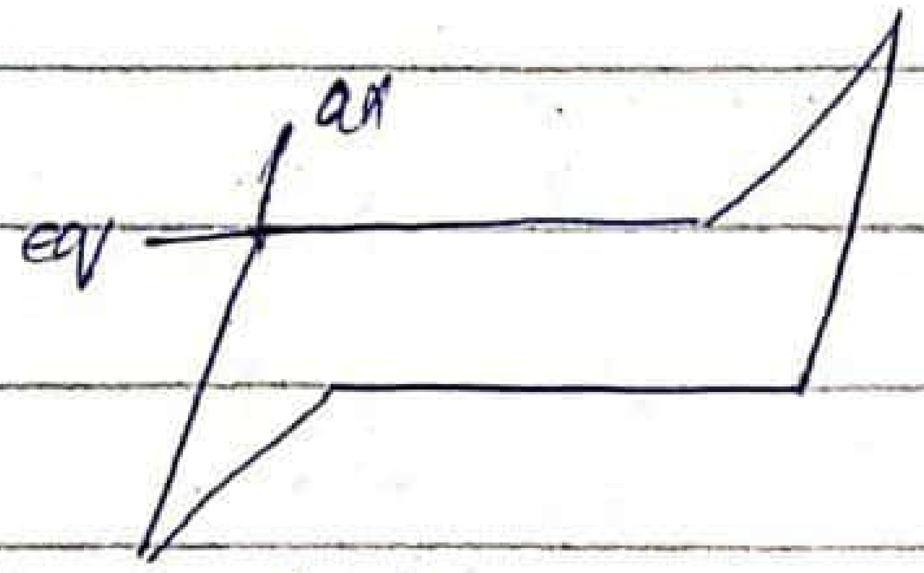


(4) Keto-Enol Tautomers:-

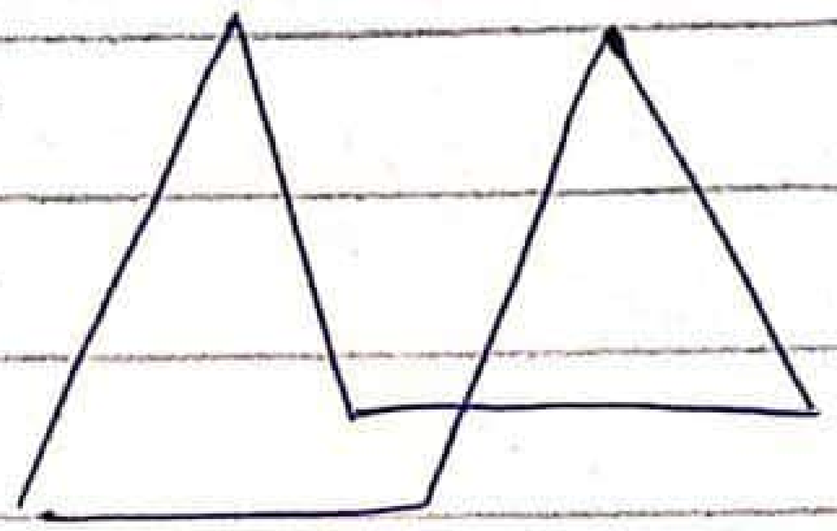
On the basis of functional group.

Keto $\longrightarrow$ Enol (OH)
(Sharp peak) will disappear (OH peak is obtained)

(5) Confirmational Isomers:-



(Chair-form)



(Boat form)

Due to equatorial & axial position that functional group is going where)

(6) Detection of Impurities:-

Additional peak.

~~Ex~~ n-Hexane + Benzene
(2900-30) Two additional peaks

(7) Forensic Science:

Criminals.

(8) Fertillizers:-

Pesticides ⟶ Organic.

(9) oil/ Fat industry:-

unsaturation /aromatic, which type of oil is present!

(10) Food industry:-

To check Toxicity.

HMF, identification is done in IR of Honey.

$C-O$, CHO ,

$C-O$, $O-H$

$C=C$, Ring = 2 peaks.

🌹 Good Luck 🌹

Practices

👇 👇 👇

IR Spectra

M JUNAID SAHOO

Lecturer Chemistry in HED (Govt. College)

🌹 🌹 🌹 🌹 🌹

Chemistry with MJS

Chemistry Preparation by MJS