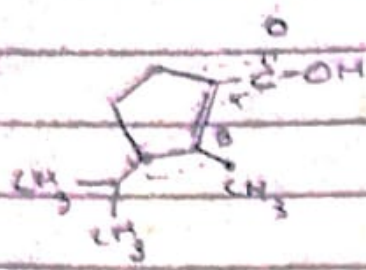


-COOH



P. value = 105 nm

Sub = $\alpha = 10$ $\beta = 24$

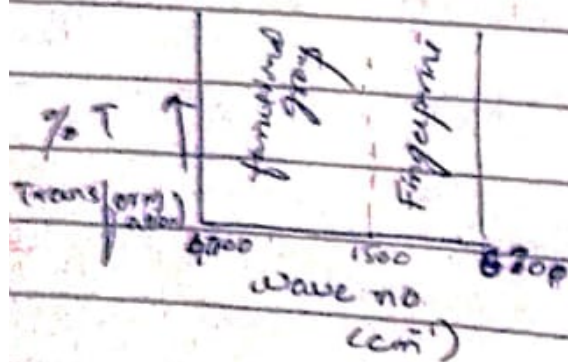
$\lambda_{max} = 229$ nm

λ_{max}

- acetaldehyde = 290 nm
- acetic acid = 208 nm
- amide -C(=O)-NH_2 = 220 nm
- Acid chloride = 220 nm

Infrared Spectroscopy (FT-IR)

- Fourier Transform Infrared Spectroscopy
- 670-4000 cm^{-1}
- Also called vibrational spectroscopy.
Because in vibrational mode of atom molecules should be observed.



- 2- Regions
- [fingerprint region (670-1500 cm^{-1})
 - [functional group region (1500-4000 cm^{-1})

⇒ In fingerprint region, provides a set of absorption band that is unique characteristic of each compound and it confirms the identity of each comp. Most of bands observed in this region is due to bending, vibration & stretching mode of molecules.

eg = C-C, C-H, C=O, C-N, C-X.

⇒ In functional group region, functional group of any org comp. can be identified which gives very strong band (absorption band) due to stretching vibration of their functional group.

eg hydrocarbon, alkane, alkene, alkyne

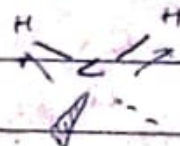
Modes of Molecules

Vibrational modes of IR

- 1- Stretching mode
- 2- Bending mode.

Symmetrical

Asymmetrical



⇒ Stretching vibration is the symmetrical movement of 2 bonded atoms along axis i.e. interatomic distance are increasing or decreasing.

If symmetrical - both stretch at one side.

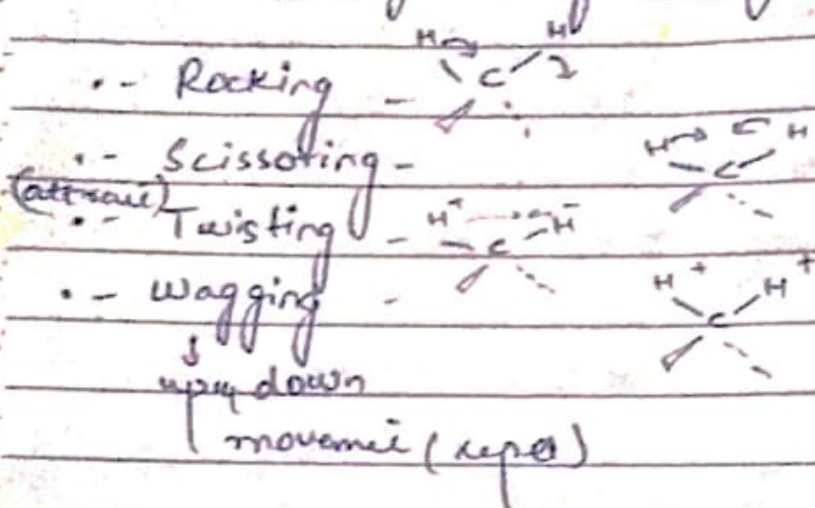
If Asymmetrical - one stretch other contract opposite side.

⇒ Bending - change in angle

↳ In this mode, change in angle b/w

2 bonds take place

4 Categories of Bending



IR ACTIVE / IR INACTIVE GROUPS

→ Active Groups are those groups of atoms, molecules or elements which gives strong peak in IR spectra.

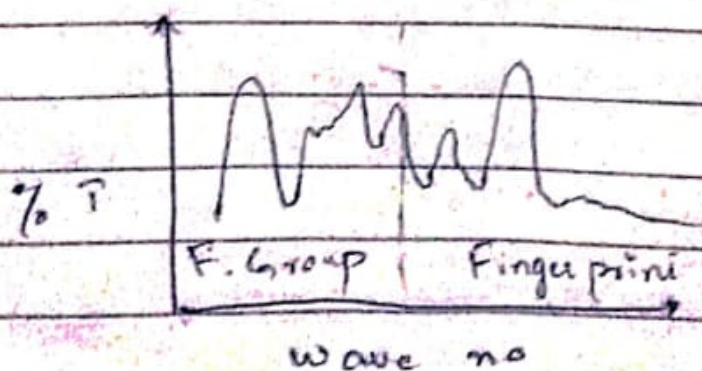
eg Carbonyl, CHO, heteroatoms - - -

Because when they absorb EMR in IR region their dipole moment changed.

→ Inactive Groups are those groups of atoms, molecules which gives weak peak.

eg H_2 , Cl_2 - - - Because ^{when} they ~~don't~~ absorb EMR in IR region their dipole moment don't change.

INTERPRETATION OF IR SPECTRA



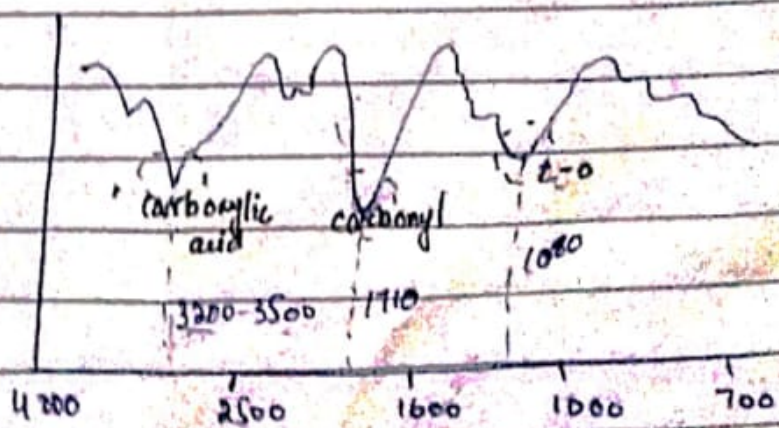
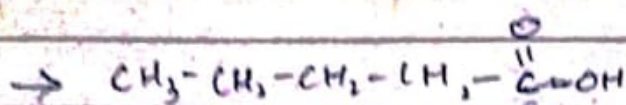
Shapes of peaks/bands

- Broad U-shaped - OH
- V-shaped - N-H (Sec Amine)
- W-shaped - NH₂ (Pri Amine)
- Sharp V - (C≡C-H) Alkyne
- Shoulder type - phenyl
- (-COOH)

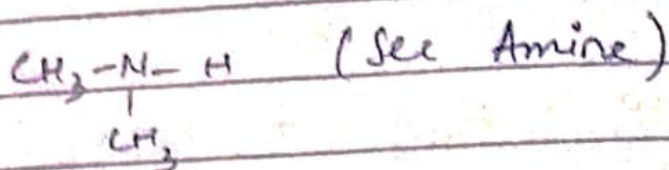
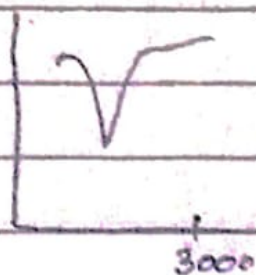
$X-H$ $N-H$ $S-H$ (Single bond) $C-H$ - 2850-3000 $O-H$ - 3200-3600 $COOH$ - 2500-3600 NH_2 - 3350-3550	Triple bond $C\equiv C$ $C\equiv N$ 2100-2260	Double bond $C=C$ (1620-1680) $C=O$ (1650-1780)	Single bond $C-C$ $C-O$ $C-H$
4000	2500	2000	1500
			600

sp^3 sp^2 sp

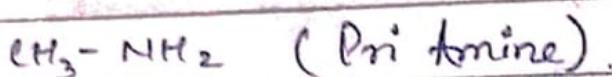
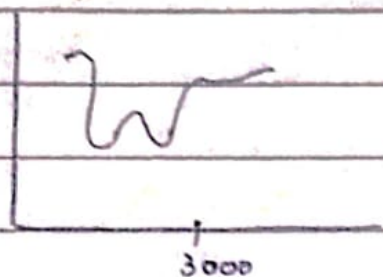
$(sp^3) C-H \rightarrow 2850-2950$ $(sp^2) =C-H \rightarrow 3000-3100$
 $(sp) \equiv C-H \rightarrow 3310-3320$



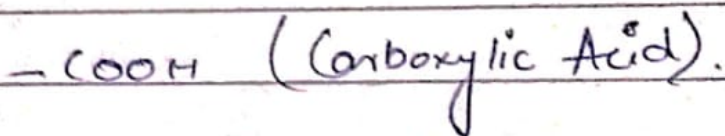
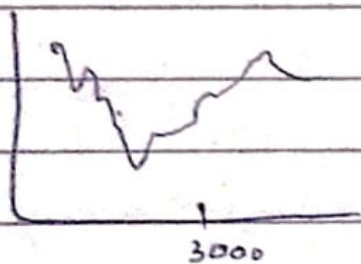
(A)



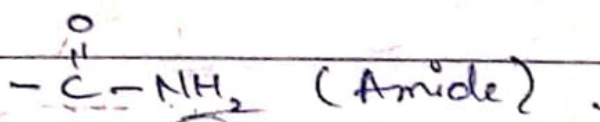
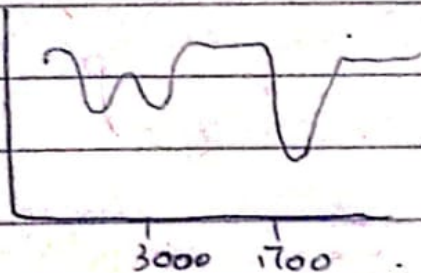
(B)

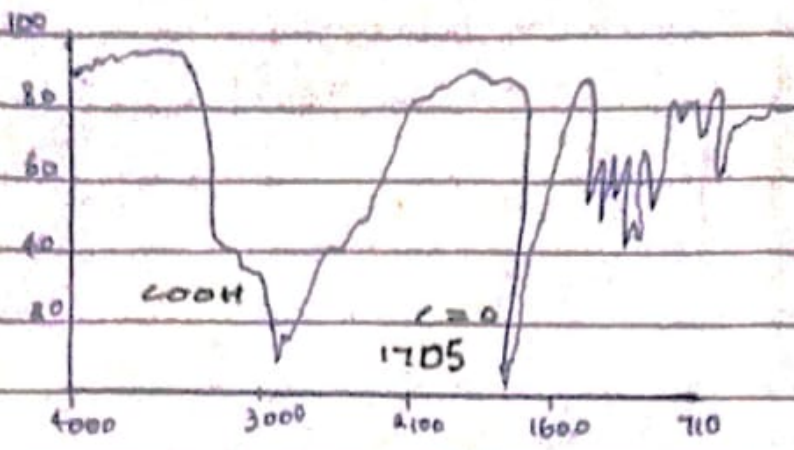
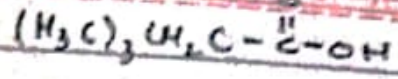


(C)

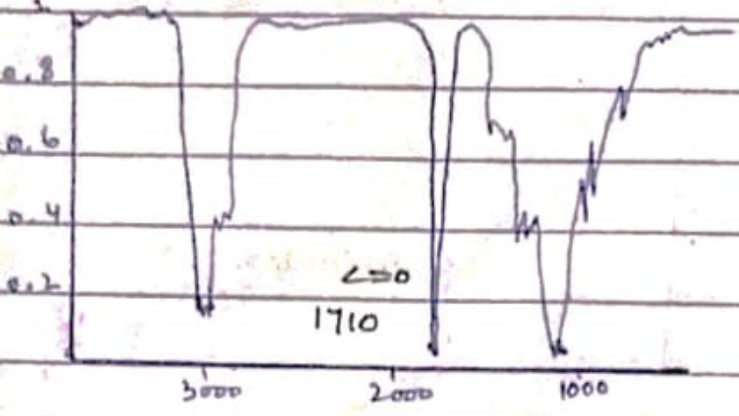
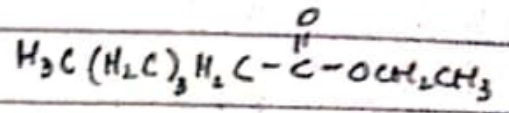


(D)

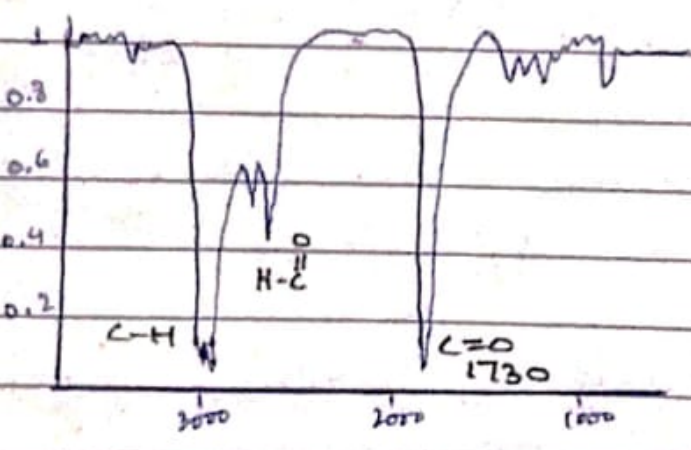
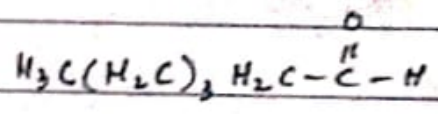




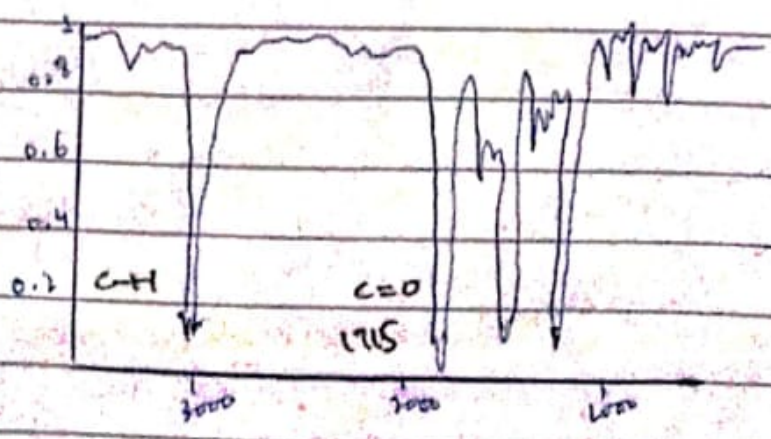
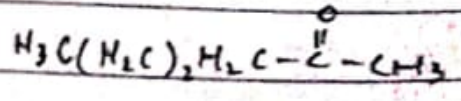
- Strong peak of C=O at 1705 cm⁻¹
- Sharp spike represent C=O
- weak peaks show stretching mode of C-H (sp³)



- Strong peak of C=O present at 1710 cm⁻¹
- At >1000 cm⁻¹ stretching mode of CH (sp³) are represent

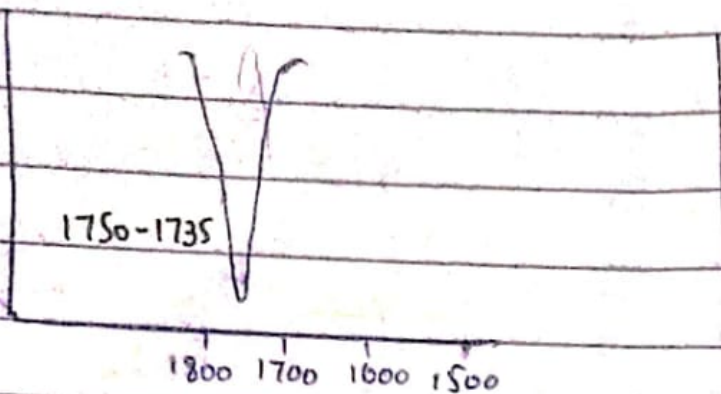


- Strong & sharp peak at 2950 cm⁻¹ represent C-H of aldehyde
- At 1730 cm⁻¹, sharp peak represent C=O of aldehyde

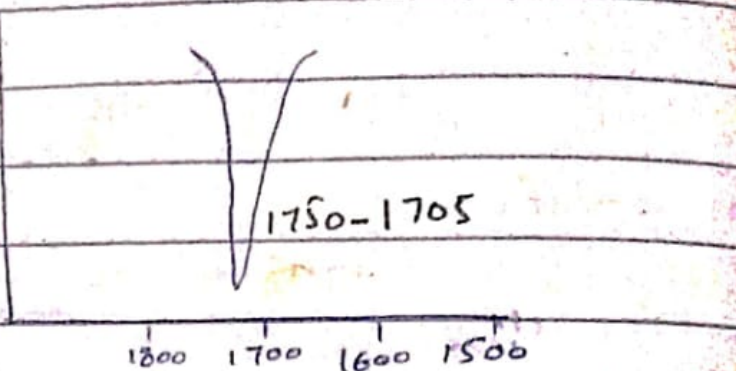


- At nearly 2950 cm⁻¹ C-H stretching sharp peak is present
- At 1715 cm⁻¹ sharp edged peak represent C=O of ketonic functional group.

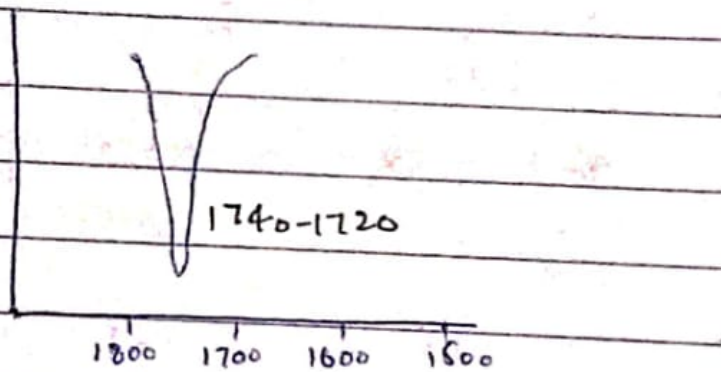
C=O (ester)



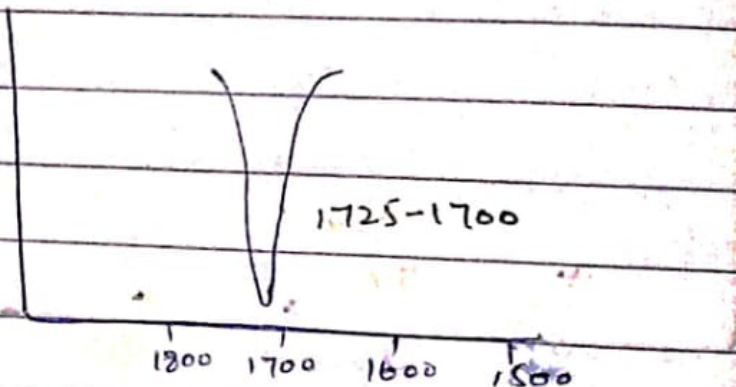
C=O (ketone)



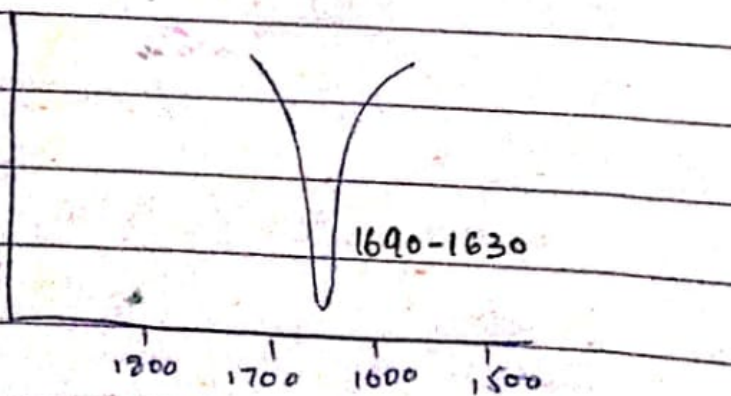
C=O (aldehyde)



C=O (carboxylic acid)



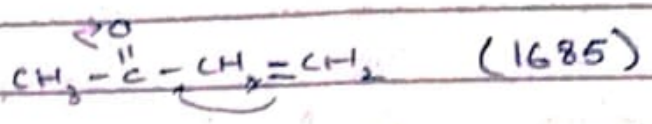
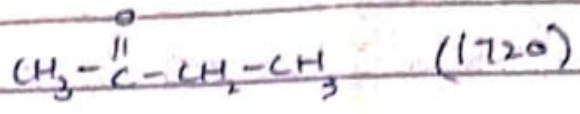
C=O (amide)



FACTORS

↓
that effect IR frequency.

• - Conjugation



e^- density ↑
freq ↓

Conjugation ↓ bond order so it decreases freq of carbonyl group.

• - Hydrogen Bonding

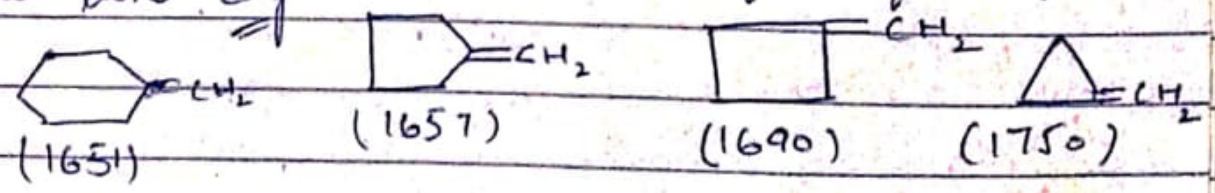
Frequency of carboxylic acid as compared to alcoholic group is lower due to hydrogen bonding.

• - Delocalization

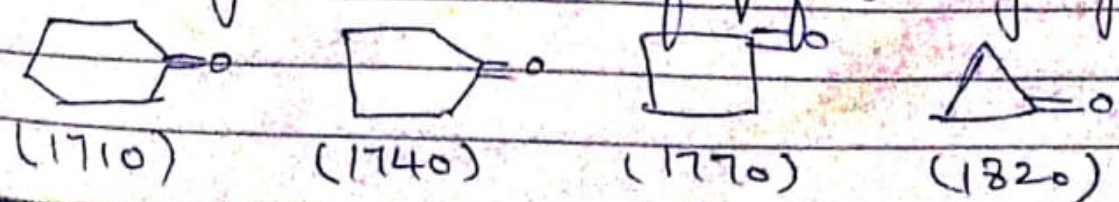
Delocalization of e^- pair decreases bond order so stretching freq. of bond also decreases.

• - Ring Strain

Ring strain increases freq. of exocyclic double bond e.g.



Ring strain increases freq. of Carbonyl group.

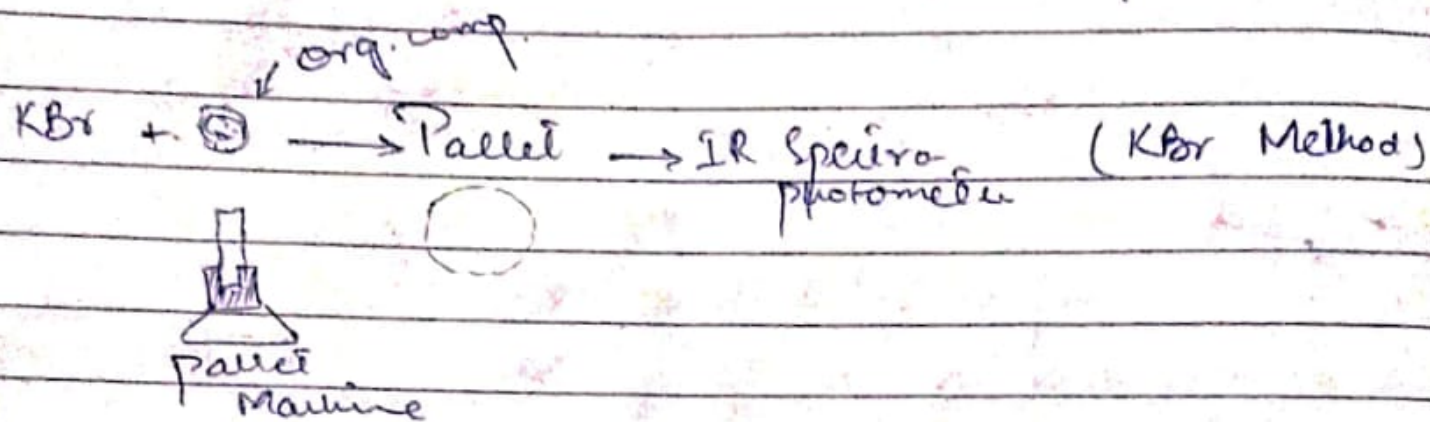


IR photometer is used to find IR spectra

By 2 - Methods

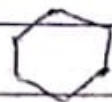
1 - KBr Method

2 - Nujol Method - Modern: pin-computer connect.



HETEROCYCLIC COMPOUNDS

Atoms other than carbon - Hetero atom.



Homo cyclic



Hetero cyclic

N, O, S - replace carbon.

5-Membered Ring



pyrrol



furan



thiol.

PYROL

→ many naturally occurring comp contain pyrrol
eg Chlorophyll & Haemoglobin, alkaloids