Ranges:- IR CONTINUE

1. O-H stretching (3600-2500 cm^{-1})
2. C-H stretching (3300-2750 cm^{-1})
3. N-H stretching (3500-3300 cm^{-1})
4. $-C\equiv C-$ stretching (2140-2100) cm^{-1} terminal
   (2260-2190) cm^{-1} internal
5. $-C\equiv N$ stretching → 2260-2100 cm^{-1}
6. C=O, C=C, C=N
   (1850-1500 cm^{-1})
   $-C=O$ (1850-1650 cm^{-1})
   C=C, $-C\equiv N$ (~1600 cm^{-1})
7. Finger print region
   (600-1500 cm^{-1})
   1500-1000 cm^{-1}
   NO_2, N=O, C-O, S=O, P=O
8. 1000-670 cm^{-1} (C-H)
   Bending vibrations (Unsaturated)
   Monosubstituted aromatic ring —
   → 770-730 cm^{-1}
   710-690 cm^{-1}
   1,2 disubstituted
   — 770-735 cm^{-1}
   1,3 → 810-750 cm^{-1}
   1,4 → 725-690 cm^{-1}

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characterstic group Vibrations :-

functional Group Region ($4000-1500 cm^{-1}$)

1) O-H stretching ($3600-2500 cm^{-1}$)

Some characteristic absorption Bands

	cm^{-1}	
1)	1050-1400	C-O (In ether, alcohol, ester)
2)	1050-1400	C-N (In amines)
3)	1315-1475	C-H (In alkanes)
4)	1340-1500	NO_2 (two peaks)
5)	1450-1600	C=C (In aromatic ring)
6)	1620-1680	C=C (In alkenes)
7)	1630-1690	C=O (In amides)
8)	1690-1750	C=O (Aldehyde, ketone, ester)
9)	1700-1725	C=O (In carboxylic acids)
10)	1770-1820	C=O (In acid chlorides)
11)	2100-2200	C≡C
12)	2210-2260	C≡N
13)	2500	S-H
14)	2700-2800	C-H (of aldehyde gp)
15)	2500-3000	O-H (of -COOH gp)
16)	3000-3100	C-H (CH part of aromatic ring)
17)	3305	C-H (C≡C)
18)	3020-3080	C-H (C=C)
19)	2800-3000	C-H (In alkanes)
20)	3300-3500	N-H (In amines) amides
21)	3200-3600	O-H (In H-bonded -OH)
22)	3600-3650	O-H

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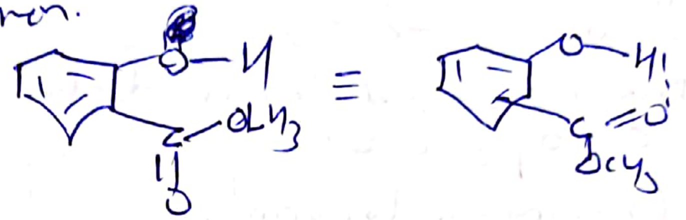
Applications of IR

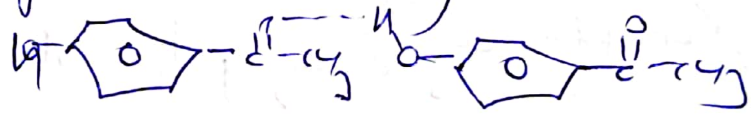
1) Detection of functional gps.
This technique can be used to identify the presence of functional groups that absorb in the region of 3500–1500 cm^{-1}

2. Effect of Different types of H-bonding
→ Intramolecular H-bonding is Independent of the conc. of sample so position of Absorption band will not vary with conc.



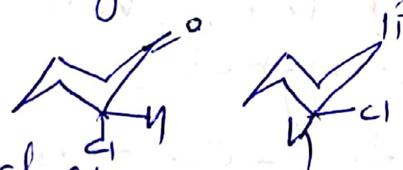
Intra molecular H-bonding

→ Intermolecular H-bonding is dependent upon conc. The more concentrated the sample, lower will be stretching frequency due to greater H-bonding



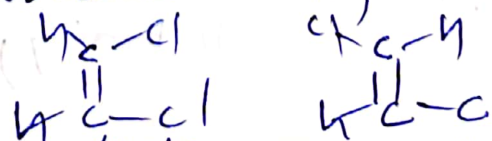
10 mg/l → C=O → 1172 cm^{-1}
20 mg/l → C=O → 1665 cm^{-1}

3.



Axial Cl — C=O 1725 cm^{-1} Equatorial Cl — C=O 1750 cm^{-1}

4. Geometrical Isomerism
C=C frequency in trans-1,2-dichloro ethylene is not observed in IR.

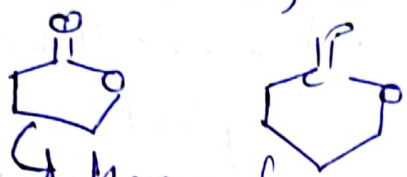


IR Inactive

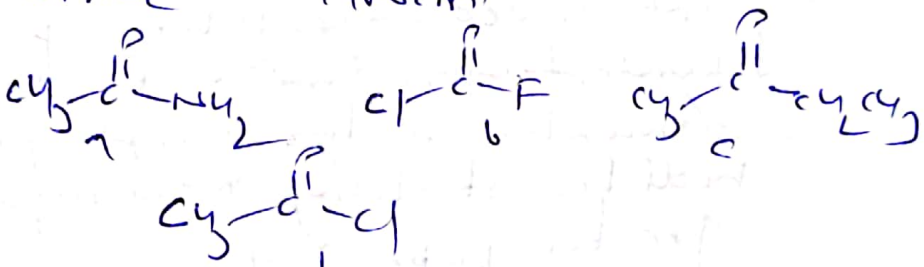
μ = 1.85 μ = 0

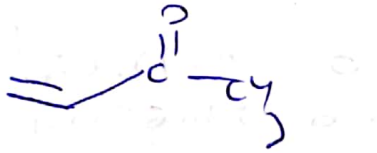
fundamentals :-

1) Relative stretching frequency of
C–C, C=C, –C≡C
C–C (1200) < C=C (1650) < C≡C (2150)

2) 
(Higher frequency C–C=O)

3) $-\overset{\overset{O}{\|}}{C}-\bar{O} \leftrightarrow -\overset{\overset{O}{\|}}{C}=O$
two CO bands Intermediate b/w C=O & C–O.
One near 1600 cm⁻¹
other 1400 cm⁻¹

4) 
(Except $CH_3-\overset{\overset{O}{\|}}{C}-NH_2$ highest in 'b')

5) 
α,β-unsaturated carbonyl absorbs at higher

6) Carboxylic acid $-\overset{\overset{O}{\|}}{C}-$ = 1760 in Vapour state, undergo intermolecular H-bonding, exist as dimers of 1680 cm⁻¹.
Vapour state – monomeric form. – 1760 cm⁻¹
Liquid/Neat – Dimerisation H-bonding, lower

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Applications of UV-Visible Spectroscopy

1. Detection of functional gp
If the spectrum of the compound is transparent above 200nm, it indicates the absence of conjugation, carbonyl gp, aromatic compound & bromo / iodo. It indicates double bond or some other atom or gp may be present

2. Extent of conjugation
Addition of unsaturation with ↑ in the no of double bonds shifts the absorption to longer wavelength.

3. Identification of an unknown compound
If the two spectra coincide, the two compounds must be identical, if not the expected structure is different from the known compound

4. Quantitative Analysis
To determine the conc of a particular compound in a soln as it is based upon Lambert-Beer law.

5. Enumeration of polynuclear hydrocarbons
Benzene & polynuclear hydrocarbons have characteristic spectra in UV-Visible region
eg Naphthalene shows absorption at 210 & 272
Anthracene → bathochromic shift

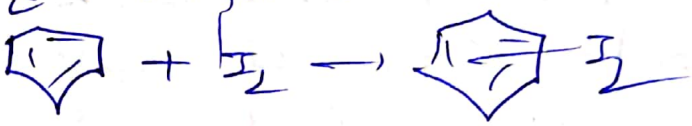
6 Determination of strength of H-bonding

Eg Acetone dissolved in benzene absorbs at 279 nm but 264 nm when dissolved in water as carbonyl compound such as acetone dissolved in polar solvent such as water,

- There is H-bond b/w solvent & $-\overset{\overset{O}{\|}}{C}-$ oxygen : Thus disruption of lower λ.

7 Study of charge transfer complex

Eg Iodine imparts Violet colour in benzene) while it is brown in benzene. This is due to formn of charge transfer complex b/w I_2 & benzene



8 Study of chemical kin

DPPH (1,1-diphenyl-2-picryl hydrazyl)

Violet colour → 515-520 nm

With antioxidant diffent

9 Keto-enol tautomerism

E.A.A keto form - 275 nm (low intensity)

enol form 245 nm

high intensity