

Class - BSc. IV Sem

Sub - Organic Chemistry

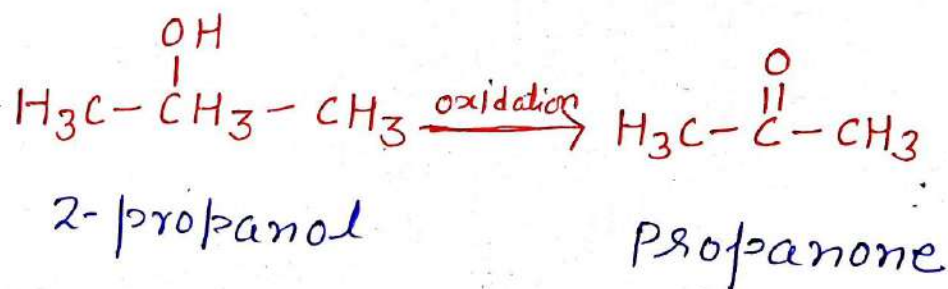
Topic - Spectroscopy

Sub-Topic - Application of IR

Application of IR Spectroscopy

(i) Study of a chemical reaction

Oxidation of 2-propanol to propanone



2-propanol gives a strong band due to hydrogen bonded O-H stretching at 3400 cm^{-1} . The oxidation will complete when a absorption band at 1700 cm^{-1} appear due to C=O stretching.

(ii) Identification of functional group

The presence and absence of absorption bands help in predicting the presence of functional groups in the compound.

Example - a carbonyl group gives IR absorption band in the range of $1690-1760\text{ cm}^{-1}$.

Bond	Type of compound	Frequency (cm^{-1})	Intensity
C-H	Alkanes	2850-2970 1340-1470	Strong
C-H	Alkenes (>C=C<^{H})	3010-3095 675-995	Medium Strong
C-H	Alkynes ($-\text{C}\equiv\text{C}-\text{H}$)	3300	Strong
C-H	Aromatic ring	3010-3100 690-900	Medium Strong
O-H	Monomeric alcohols, phenols	3590-3650	Variable
	Hydrogen bonded alcohols, phenols	3200-3600	Variable
	Monomeric carboxylic acids	3500-3650	Medium
	Hydrogen bonded carboxylic acids	2500-2700	Broad
N-H	Amines, amide	3300-3500	Medium
C=C	Alkenes	1610-1680	Variable
C \equiv C	Alkynes	2100-2260	Variable
C-N	Amines, amides	1180-1360	Strong
C \equiv N	Nitriles	2210-2280	Strong
C-O	Alcohols, Esters, ethers carboxylic acids, esters	1050-1300	Strong
C=O	Aldehyde, ketones, esters carboxylic acids	1690-1760	Strong
NO ₂	Nitro compounds	1500-1570 1300-1370	Strong

(iii) Purity of a compound

A pure compound has well-defined and sharp absorption frequencies whereas the spectra of Impure compound has diffused and blurred due to impurity present in the sample.

(iv) Determination of structure

IR spectroscopy helpful to determine the structure

Example - The absorption frequencies of a compound as follow -

Aromatic C-H stretching - $3060, 3030, 3000 \text{ cm}^{-1}$

Methyl C-H stretching - $2950, 2835 \text{ cm}^{-1}$

Overtone - $2000-1650 \text{ cm}^{-1}$

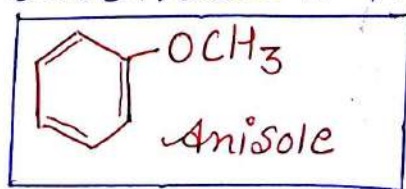
C=C stretching - $1590, 1480 \text{ cm}^{-1}$

C-O-C stretching - $1245, 1030 \text{ cm}^{-1}$

C-H bending - $800, 740 \text{ cm}^{-1}$

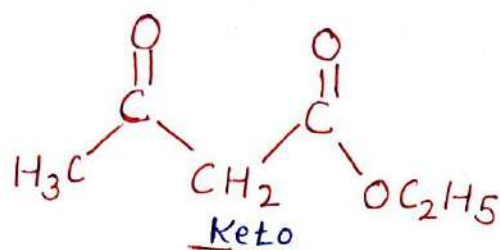
C=C bending - 680 cm^{-1}

Based on the above observation the compound is Anisole



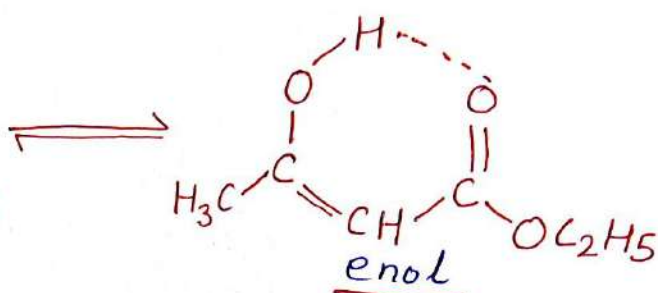
(V) Study of Keto-Enol tautomerism

Ethyl acetoacetic ester exists in keto-enol isomers in equilibrium.



$\nu_{C=O}$ str.

$1733, 1710 \text{ cm}^{-1} (s)$



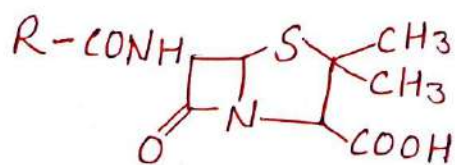
ν_{O-H} str. $3300 \text{ cm}^{-1} (b)$

$\nu_{C=O}$ str. $1645 \text{ cm}^{-1} (s)$

Lowering of $\nu_{C=O}$ str. absorption in enolic form is due to intra-molecular hydrogen bonding which is established by resonance.

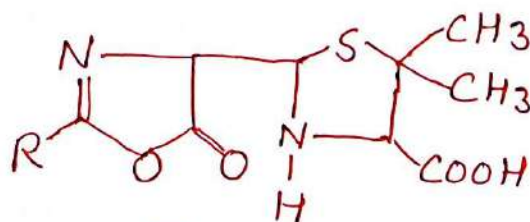
(VI) Study of complex Molecules

Two structures of Penicillin were proposed on the basis of IR spectral studies.



I

β -Lactam str.



II

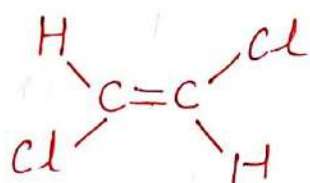
Oxazolone str.

IR spectra of oxazolone show $\nu_{C=O}$ str. due to 1825 cm^{-1} and $\nu_{C=N}$ str. due to 1675 cm^{-1} . These bands not found in IR spectrum of Penicillin. So, Oxazolone structure for Penicillin is ruled out.

(VIII) Geometrical Isomerism

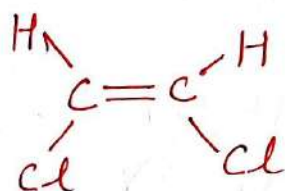
Intensity of absorption depends upon the change in the dipole moment. This technique distinguishes between cis and trans isomers.

Geometrical isomers of 1,2-dichloroethene



Trans

($\mu=0$)



cis

($\mu=1.85 \text{ D}$)

$\text{C}=\text{C}$ stretching at 1580 cm^{-1} is not observed in case of trans isomers since the vibration does not change in dipole moment. This peak (1580 cm^{-1}) appears due to $\text{C}=\text{C}$ str. in cis isomer.

Reference

"Elementary Organic Spectroscopy" Principles and chemical Applications Published S. Chand by Y.R. Sharma