Seat No. : _______________

NH-137

November-2025

M.Sc., Sem.-III

CHE (O) – 503 : Organic Chemistry

(Organic Spectroscopy)

Time : 2:30 Hours] **[Max. Marks : 70**

1. (A) Discuss the different types of spectral shifts in UV Spectroscopy. 7

   (B) Discuss the different types of vibrational modes observed in IR spectra. 7

OR

1. (A) Discuss effect of H-bond on IR frequencies and role of IR to distinguish different types of H-bond. 7

   (B) Discuss the selection of solvent in UV Spectroscopy. 7

2. (A) Discuss the use of shift reagents with suitable examples in ^{1}H NMR Spectroscopy. 7

   (B) Discuss off-resonance decoupling technique in ^{13}C NMR Spectroscopy. 7

OR

2. (A) Write short notes on 2D HETCOR 7

   (B) Discuss spin-spin splitting and explain vicinal and long-range coupling. 7

3. (A) Describe the Chemical Ionization (CI) technique in mass spectrometry. 7

   (B) Discuss the fragmentation of propanol and propanal in mass spectra. 7

OR

3. (A) Describe rearrangement reactions occurring during fragmentation in Mass spectrometry. 7

   (B) Discuss principle and application of mass spectrometry. 7

4. (A) An organic compound with molecular formula $C_9H_{11}NO_2$ exhibits following spectral data : 7

   IR : 3380, 3460, 3010, 2985, 1708, 1622, 1600, 1575, 1465, 1382, 1225, 1095, 822 cm^{-1}

   1H NMR (δ ppm): 1.30 (3H, t), 4.0 (2H, br), 4.29 (2H, q), 6.57 (2H, d), 7.72 (2H, d)

   13C NMR (δ ppm): 14, 61, 116, 119, 129, 147, 167

   Mass(m/z): 165, 136, 120, 92, 65, 29

   Deduce the structure of compound with suitable explanation.

(B) An organic compound with molecular formula $C_3H_5BrO_2$ exhibits following spectral data : **7**

UV : λmax 223 nm

IR : 3125-2599, 1718, 1420, 1092, 735 cm^{-1}

^1H NMR (δ ppm) : 1.9 (3H, d), 4.4 (1H, quartet), 11.6 (1H, s)

^{13}C NMR(δ ppm) : 21, 42, 176

Deduce the structure of compound with suitable explanation.

OR

4\. (A) Deduce the structure with explanation of a hydrocarbon with following spectral data : **7**

IR: 3021, 2942, 2892, 1604, 1582, 1469, 1388, 756 cm^{-1}

^1H NMR (δ ppm): 2.1 (2H, quintet), 2.9 (4H, t), 7.2 (4H, complex)

^{13}C NMR (δ ppm): 25.3, 32.89, 124.2, 126, 144

Molecular ion peak: 118 m/z

(B) An organic compound containing 85.7 % C and 14.3 % H gave the following spectral data : **7**

UV: Transparent above 210 nm

IR: 3020, 2958, 1657, 1585 and 965 cm^{-1}.

^1H NMR : 8.40 τ (Doublet), 4.45 τ (quartet) (ration of 3:1)

^{13}C NMR (δ ppm): 15, 128

Mass (m/z): 56, 41, 27, 15

Deduce the structure of compound with suitable explanation.

5\. Answer the following questions in short (any **seven**) : **14**

(1) What is meant by fingerprint region in IR spectra ?

(2) Define auxochrome with one example.

(3) Name any two types of light sources used in UV-Visible spectroscopy

(4) Mention two important applications of IR spectroscopy in organic chemistry.

(5) Write number of ^1H NMR peak of 2-bromobutane.

(6) Why is ^{13}C NMR less sensitive than ^1H NMR ?

(7) What type of correlations are observed in COSY spectra ?

(8) What is the main advantage of DEPT spectra ?

(9) Define : Metastable peak

(10) What is the characteristic peak pattern observed in the mass spectrum of a compound containing one bromine atom ?

(11) What does a peak at m/z 91 typically indicate in aromatic compounds ?

(12) Why does cyclohexane give a single signal at room temperature but two signals at low temperature ?

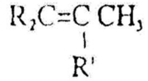
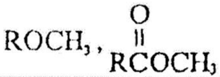
SELECTED SPECTRAL DATA

Characteristic Infrared Absorption Frequencies

Bond Type	**Stretching, cm^{-1}**	**Bending, cm^{-1}**
C-H alkanes	2960-2850 (s)	1470-1350 (s)
C-H alkenes	3080-3020 (m)	1000-675 (s)
C-H aromatic	3100-3000 (v)	870-675 (v)
C-H aldehyde	2900, 2700 (m, 2 bands)	
C-H alkyne	3300(s)	
C≡C alkyne	2260-2100 (v)	
C≡N nitrite	2260-2220 (v)	
C=C alkene	1680-1620 (v)	
C=C aromatic	1600-1450 (v)	
C=O ketone	1725-1705 (s)	
C=O aldehyde	1740-1720 (s)	
C=O α,β-unsaturated ketone	1685-1665 (s)	
C=O aryl ketone	1700-1680 (s)	
C=O ester	1750-1735 (s)	
C=O acid	1725-1700 (s)	
C=O amide	1690-1650 (s)	
O-H alcohols (not hydrogen bonded)	3650-3590 (v)	
O-H alcohols (hydrogen bonded)	3600-3200 (s, broad)	1620-1590 (v)
O-H acids	3000-2500 (s, broad)	1655-1510 (s)
N-H amines	3500-3300 (m)	
N-H amides	3500-3350 (m)	
C-O alcohols, ethers, esters	1300-1000 (s)	
C-N amines, alkyl	1220-1020 (w)	
C-N amines, aromatic	1360-1250 (s)	
NO_2 nitro	1560-1515 (s)	
	1385-1345 (s)	

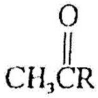
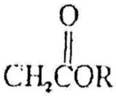
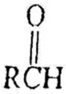
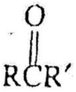
s = strong absorption
w = weak absorption
m = medium absorption
v = variable absorption

Typical chemical shifts for Types of Hydrogen Atoms, Seen in Proton Magnetic Resonance Spectra

Type of Hydrogen Atom	δ*	Type of Hydrogen Atom	δ*
RCH_3	0.9	$R_2C{=}CH_2$	5.0
RCH_2R acyclic	1.3	$RCH = CR_2$	5.3
acyclic	1.5	ArH	7.3
R_3CH	1.5–2.0	 $R\overset{O}{\overset{\Vert}{C}}H$	9.7
 $R_2C{=}\underset{R'}{\underset{\vert}{C}}CH_3$	1.8	RNH_2	1-3
 $R\overset{O}{\overset{\Vert}{C}}CH_3$	2.0–2.3	$ArNH_2$	3-5
$ArCH_3$	2.3	 $R\overset{O}{\overset{\Vert}{C}}NHR$	5-9
RC≡CH	2.5	ROH	1-5
$RNHCH_3$	2–3	ArOH	4-7
$RCH_2X(X = Cl, Br, I)$	3.5	 $R\overset{O}{\overset{\Vert}{C}}OH$	10-13
 $ROCH_3$, $R\overset{O}{\overset{\Vert}{C}}OCH_3$	3.8		

52	C_4H_4, C_2N_2
53	C_4H_5
54	$CH_2 = CH - CH = CH_2$
55	$CH_2 = CHCHCH_3$
56	$CH_2 = CHCH_2CH_3$, $CH_3CH = CHCH_3$, 2CO
57	C_4H_9· (butyl ketones), C_2H_5CO (ethyl ketones, EtC=OG, G = various structural units)
58	·NCS, (NO + CO), CH_3COCH_3, C_4H_{10}

Chemical Shifts for Carbon Atoms in Carbon - 13 Nuclear Magnetic Resonance Spectra

Type of Carbon Atom	δ*	Type of Carbon Atom	δ*
RCH_2CH_3	13–16	$RCH = CH_2$	115–120
RCH_2CH_3	16–25	$RCH = CH_2$	125–140
R_3CH	25–38	$RC \equiv N$	117–125
 $CH_3\overset{O}{\overset{\|}{C}}R$	~30	ArH	125–150
 $CH_2\overset{O}{\overset{\|}{C}}OR$	~20	 $R\overset{O}{\overset{\|}{C}}OR'$	170–175
RCH_2Cl	40–45	 $R\overset{O}{\overset{\|}{C}}OH$	177–185
RCH_2Br	28–35	 $R\overset{O}{\overset{\|}{C}}H$	190–200
RCH_2NH_2	37–45	 $R\overset{O}{\overset{\|}{C}}R'$	205–220
RCH_2OH	50–64		
$RC \equiv CH$	67–70		
$RC \equiv CH$	74–85		