Seat No. : _____

MC-102

March-2025

M.Sc., Sem.-III

CHE(O)-503 : Organic Chemistry (Organic Spectroscopy)

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

1. (A) Discuss different shifts in UV spectroscopy. **7**
1. (B) Discuss solvents effect in UV spectroscopy. **7**

OR

1. (A) Discuss the preparation method for samples for IR spectroscopy. **7**
1. (B) Discuss the various applications of IR spectroscopy. **7**

2. (A) Discuss the coupling constant (J) in 1H NMR spectroscopy. **7**
2. (B) Discuss the various applications of 1H NMR spectroscopy. **7**

OR

2. (A) Give the differences between 13C NMR and 1H NMR. **7**
2. (B) Write a note on 2D NMR spectroscopy. **7**

3. (A) Discuss Electron Spray Ionization (ESI) techniques for mass spectrometry. **7**
3. (B) Discuss the various types of peaks in mass spectrometry. **7**

OR

3. (A) Discuss MALDI techniques for mass spectrometry. **7**
3. (B) Discuss the mass spectra of ketones with examples. **7**

4. (A) An organic compound with molecular formula $C_7H_{12}O_2$ exhibits following spectral data : **7**

IR (cm^{-1}) : 3050, 2980, 2900-2200 (broad peak), 1250

1H NMR (δ ppm) : 0.93 (6H, d), 2.05 (1H, m), 2.85 (1H, t), 5.21 (2H, d), 5.94 (1H, q), 12.22 (1H, s)

13C NMR (δ ppm) : 19, 32, 55, 114, 138, 178

Mass (m/z) : 128.08

Deduce the structure of the compound with suitable explanation.

4. (B) An organic compound with molecular formula C_6H_8O exhibits following spectral data : **7**

IR (cm^{-1}) : 3400, 3040, 2990, 1250

1H NMR (δ ppm) : 0.8 (3H, d), 3.0 (1H, hex), 6.3 (1H, s), 6.4 (1H, d), 6.5 (1H, d), 10.7 (1H, s)

13C NMR (δ ppm) : 21, 30, 120, 134, 151, 181

Mass (m/z) : 96.06

Deduce the structure of the compound with suitable explanation.

OR

4. (A) An organic compound with molecular formula C_7H_9NO exhibits following spectral data : **7**

IR (cm^{-1}) : 3310, 3411, 3092, 2979, 1258, 1198

1H NMR (δ ppm) : 3.74 (3H, s), 5.22 (2H, s), 6.29 (1H, d), 6.32 (1H, d), 6.44 (1H, s), 7.10 (1H, t)

13C NMR (δ ppm) : 56, 102, 107, 111, 130, 151, 161

Mass (m/z) : 123.07

Deduce the structure of the compound with suitable explanation.

4. (B) An organic compound with molecular formula $C_9H_9NO_3$ exhibits following spectral data : **7**

IR : 3040, 2980, 1740, 1600, 1500, 1200

1H NMR (δ ppm) : 1.2 (3H, t), 3.0 (2H, q), 8.3 (2H, d), 8.4 (2H, d)

13C NMR (δ ppm) : 9, 31, 124, 130, 142, 152, 200

MS : 179.06 (100%), 180.06 (10.3%)

Deduce the structure of the compound with suitable explanation.

5. Answer any **seven** out of **twelve** : **14**

(i) Write the range for vacuum UV spectroscopy and visible spectroscopy.

(ii) Define chromophore.

(iii) Name the forbidden transitions in UV-visible spectroscopy.

(iv) Discuss the importance of Deuterium exchange with an example in NMR spectroscopy.

(v) What is the full form of NOESY ?

(vi) Explain whether 31P nuclei is NMR active, with a reason.

(vii) What is the full form of DEPT NMR ?

(viii) What are bromine's characteristic peaks in mass spectrometry ?

(ix) What are the full form of FD and FID ionization techniques ?

(x) Define characteristic peak for cyanide group in functional group region for IR spectroscopy.

(xi) Explain the characteristic peaks for prop-1-yne in IR spectroscopy.

(xii) Calculate degrees of freedom in aniline molecule.

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	$\begin{matrix}O\\\|\\RCH\end{matrix}$	9.7
$R_2C=C(R')CH_3$	1.8	RNH_2	1–3
$\begin{matrix}O\\\|\\RCCH_3\end{matrix}$	2.0–2.3	$ArNH_2$	3–5
$ArCH_3$	2.3	$\begin{matrix}O\\\|\\RCNHR\end{matrix}$	5–9
$RC\equiv CH$	2.5	ROH	1–5
$RNHCH_3$	2–3	ArOH	4–7
RCH_2X(X = Cl, Br, I)	3.5	$\begin{matrix}O\\\|\\RCOH\end{matrix}$	10–13
$ROCH_3$, $\begin{matrix}O\\\|\\RCOCH_3\end{matrix}$	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
$CH_3\overset{\overset{O}{\|}}{C}R$	~30	ArH	125–150
$CH_2\overset{\overset{O}{\|}}{C}OR$	~20	$R\overset{\overset{O}{\|}}{C}OR'$	170–175
RCH_2Cl	40–45	$R\overset{\overset{O}{\|}}{C}OH$	177–185
RCH_2Br	28–35	$R\overset{\overset{O}{\|}}{C}H$	190–200
RCH_2NH_2	37–45	$R\overset{\overset{O}{\|}}{C}R'$	205–220
RCH_2OH	50–64		
$RC \equiv CH$	67–70		
$RC \equiv CH$	74–85		