2203N1705

Candidate's Seat No :_____

M.Sc. Semester-3 Examination

503

Chemistry (O)

March-2024

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

Q. 1 (A) Discuss the different electronic transitions in UV spectroscopy. 07

(B) Describe instrumentation for UV spectroscopy. 07

OR

(A) Explain the preparation method for samples for IR spectroscopy. 07

(B) Discuss the various mode of vibrations in IR spectroscopy. 07

Q. 2 (A) What is coupling constant? Discuss various types of coupling constant. 07

(B) Discuss HETCOR NMR spectroscopy. 07

OR

(A) What information can be derived from an NMR spectrum? 07

(B) Explain in detail: 07

1. Explain the reasons for using TMS as a standard in NMR analysis.
2. COSY in 1H NMR

Q. 3 (A) Discuss Electrospray ionization techniques for mass spectrometry. 07

(B) Discuss the Mc-Lafferty rearrangement with two examples for mass spectrometry. 07

OR

(A) Define it: Parent peak, Base peak, Molecular ion peak and Metastable peak. 07

(B) Write the applications of mass spectral data. 07

Q. 4 (A) An organic compound with molecular formula C_7H_7NO exhibits following spectral data: 07

IR (cm^{-1}): 3400, 3300, 3060, 2980, 1690, 1100

1H NMR (δ ppm): 7.45 (2H, t), 7.66 (1H, t), 7.70 (2H, s), 7.77 (2H, d)

13C NMR (δ ppm): 125, 128, 132, 134, 168

Deduce the structure of the compound with suitable explanation.

(B) An organic compound with molecular formula C_5H_6O exhibits following spectral data: 07

IR (cm^{-1}): 3300, 3050, 2960, 1500, 1130

1H NMR (δ ppm): 4.75 (1H, s), 5.00 (1H, t), 6.40 (2H, t), 6.50 (2H, t)

13C NMR (δ ppm): 75, 130, 132

MS: 82.04 (100%), 83.05 (5.5%)

Deduce the structure of the compound with suitable explanation.

OR

(A) An organic compound with molecular formula $C_{10}H_{12}O$ exhibits following spectral data: 07

IR (cm^{-1}): 3023, 3285, 1730, 1550

1H NMR (δ ppm): 1.20 (6H, d), 3.20 (1H, m), 7.50 (2H, d), 7.85 (2H, d), 9.90 (1H, s)

13C NMR (δ ppm): 23, 33, 126, 130, 135, 152, 190

MS: 148.09 (100%), 149.09 (10.9%)

Deduce the structure of the compound with suitable explanation.

P.T.O

(B) An organic compound with molecular formula $C_4H_9NO_3$ exhibits following spectral data: 07

IR (cm^{-1}): 3600, 3500, 3400, 2980, 2500-2900, 1720

1H NMR (δ ppm): 1.20 (2H, q), 3.40 (1H, t), 3.80 (2H, t), 4.40 (1H, s), 8.50 (2H, s), 12.40 (1H,s)

13C NMR (δ ppm): 38, 51, 58, 175

MS: 119.06 (100%), 120.06 (4.9%)

Deduce the structure of the compound with suitable explanation.

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

(i) Write the full form of HOMO and LUMO.

(ii) Explain blue shifts in UV spectroscopy.

(iii) Discuss characteristic peaks for amide group in functional group region for IR spectroscopy.

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

(v) Which organic compound with molecular formula $C_3H_6Cl_2$ exhibits only one signal in the IH NMR spectrum?

(vi) Explain: The nitrogen rule in mass spectrometry.

(vii) Define down-field region in 1H NMR spectroscopy.

(viii) What is chlorine's characteristic peaks in mass spectrometry?

(ix) Write the full form of HRMS.

(x) Write range for 13C NMR spectroscopy with unit.

(xi) What is the abundance of 13C and 12C isotopes?

(xii) Write the possible electronic transition in acetaldehyde.

N1705-3

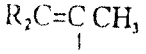
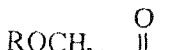
SELECTED SPECTRAL DATA

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
m = medium absorption
w = weak 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		9.7
	1.8	RNH_2	1–3
	2.0–2.3	$ArNH_2$	3–5
$ArCH_3$	2.3		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		10-13
	3.8		

(P.T.O)

N 1705-4

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		