

DEPARTMENT OF CHEMISTRY
SCHOOL OF CHEMICAL & LIFE SCIENCES
M.SC. CHEMISTRY
SEMESTER-II EXAMINATION-2023
PAPER TITLE: APPLICATIONS OF SPECTROSCOPY
PAPER CODE: MCHCC – 204

Time 2 Hours

Maximum Marks 60

Note: This paper has 3 sections A, B, and C, Attempt all the three sections

Section A: Answer all the questions; Section B: Answer any 2 out of 4; Section C: Answer all the questions, each question has an internal choice.

Abbreviations Used:

CLO- Course Outcome, PLO- Program Outcome, BTL- Bloom Taxonomy Level: BT level1-Remember; BT level 2-Understand; BT level 3-Apply; BT level 4-Analyse; BT level 5-Evaluate, BT level 6-Create

SECTION A

(10x2 = 20 Marks)

Q.	Very short type questions (Attempt All)	BTL	CLO	PLO
A 1.	What is the distance between the centers of the peaks of a multiplet in the NMR spectrum called? What does the splitting depend on and what information can it give us?	2/3	1/3	1/2
A 2.	An IR spectrum is taken before and after treating acetone with the reducing agent NaBH ₄ . What IR peak readings would be seen for the reactant acetone and for the predicted product?	3/4	3/4	2
A 3.	How many peaks will be observed in the signals due to the circled hydrogens in the ¹ H-NMR spectra of the following compounds? a. b. c.	3/4	3/4	3/4
A 4.	Which of the following compounds show a strong absorption at ~1700 cm ⁻¹ and a broad absorption at 2500 – 3300 cm ⁻¹ in its IR spectrum? Or	1/3	2	2
A 5.	What is the order of vibrational frequency for C — Cl, C — Br, C — C, C — O and C — H bonds in IR spectroscopy and why?	1/2	2-4	2
A 6.	What class of compounds is most likely to give a fragment ion at m/z = M-18 in its MS?	1/3	3-5	3/4
A 7.	A conjugated diene has a λ _{max} , 219 nm in hexane. What will happen to λ _{max} if solvent is changed to ethanol?	1/2	2/3	4
A 8.	Acetone absorbs light at 280, 187 and 154 nm. Which are the transitions responsible for each of these absorptions?	2/3	3/4	4
A 9.	What characterization information is obtained from out-of-plane bending C-H absorptions in an IR spectrum?	2/3	3/4	5
A 10.	How many peaks can be seen in the ¹ HNMR spectrum of the following compound? CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	2/3	3/4	5

SECTION B

(10x2 = 20 Marks)

Q.	Long-type questions (Attempt any two out of four)	BTL	CLO	PLO
B 1.	A) What is the structure of a compound C₉H₁₀O that has an IR absorption at 1688 cm⁻¹ and ¹HNMR signals at 1.22 (triplet, 3H), 2.98 (quartet, 2H), and 7.28-7.95 (multiplet, 5H)? B) Use Woodward-Fieser Rules to predict λ_{max} of the following i) ii) iii) iv) v)	2/3	1/3	1/2

B 2.	A) What is the principle of Raman spectroscopy? How does this technique complement IR spectroscopy B) What is Attenuated Total Reflectance (ATR) and how can it be used for samples of different nature?	3/4	3/4	2
B 3.	A) What is the significance of the 2D techniques, COSY, HETCOR and HMBC? B) Why are Spin-Spin relaxation and Spin Lattice relaxation important for NMR signals?	1	2	3/4
B 4.	Deduce the identity of the following compounds from the spectral data given i. $C_4H_{10}O$: ^{13}C data: δ 10.0 (quartet), 22.9 (quartet), 32.0 (triplet), 69.6 (doublet) ii. $C_7H_{14}O_2$: 1H NMR (d): 2.3 (2H, q), 1.0 (3H, t), 0.9 (9H, s); ^{13}C NMR (d): 185 (s), 78 (s), 29 (t), 14 (q), 12 (q), IR (cm^{-1}): 2950, 1740; IR (cm^{-1}): 2950, 1740 iii. C_3H_4BrN : 1H NMR, δ 2.98 (2H, triplet), 3.53 (2H, triplet); ^{13}C NMR, δ 21.05 (triplet), 23.87 (triplet), 118.08 (singlet); IR, 2963, 2254 cm^{-1})	1/3	2	2

SECTION C

(5x4 = 20 Marks)

Q.	Short-type questions. (Attempt all the questions)	BTL	CLO	PLO
C 1.	Differentiate between the following on the basis of IR <chem>OCc1ccccc1</chem> OR The absorbance values of a mixture of $K_2Cr_2O_7$ and $KMnO_4$ at 430 nm and 540 nm using a cell of 1 cm path length were found to be 0.461 and 0.123 respectively. The absorbance values of pure solutions of $K_2Cr_2O_7$ (0.001 M) and $KMnO_4$ (0.0002 M) in similar conditions were as follows: $A(Cr, 440\text{ nm}) = 0.214$, $A(Cr, 545\text{ nm}) = 0.001$ $A(Mn, 440\text{ nm}) = 0.020$, $A(Mn, 545\text{ nm}) = 0.375$ Using the given data determine the concentration of $Cr_2O_7^{2-}$ ions and MnO_4^- ions in the mixture. <chem>COc1ccccc1</chem>	2/3	1/3	1/2
C 2.	Predict the approximate positions of all of the important absorptions in the IR spectrum of these two compounds. <chem>CH3CH2CH=CHCOOH</chem> OR What are the Variables that affect the fluorescence signal of a compound? How can the quantum yield be improved? <chem>CC(=O)Cc1ccccc1</chem>	3/4	3/4	2
C 3.	Discuss how diamagnetic and paramagnetic components contribute to shielding in NMR? OR Is it possible to identify the following classes of compounds by their infrared (IR) spectra? And if so, how? Ester, aldehyde, ketone, nitrile, Carboxylic acid	1	2	3/4
C 4.	The McLafferty rearrangement is one of the important pathways of alkene loss from molecular ions. Justify with examples OR A) A liquid compound gave a mass spectrum showing a strong molecular ion at $m/z = 156$. The only fragment ions are seen at $m/z = 127$ & 29. Suggest a structure for this compound B) The mass spectrum of 2-butenal shows a peak at m/z 69 that is 28.9% as intense as the base peak. Propose a fragmentation route to account for this peak and explain why this fragment would be reasonably stable	1/3	2	2
C 5.	How are the following ionization methods used in Mass spectrometry different 1. Electron Impact 2. Chemical Ionization 3. FAB 4. Electrospray ionization OR Predict the number of signals expected in the proton spin decoupled ^{13}C spectrum of the following i. 3-pentanone ii. 1,3-dichlorobenzene iii. 1,4-dibromobenzene iv. Cyclopentane v. cis-1,3-dimethylcyclopentane	1/2	2-4	2