Reg. No ..... Name **25P344-S**

M. Sc. DEGREE END SEMESTER EXAMINATION - OCTOBER 2025

SEMESTER 3 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

COURSE : **21P3CHET12 / 21P3CPHT12 : SPECTROSCOPIC METHODS IN CHEMISTRY**

(For Supplementary 2023/ 2022/2021 Admissions)

Time : Three Hours Max. Weights: 30

PART A

Answer any 8 questions **Weight: 1**

1.	An unknown organic compound with MF C_4H_5NO displays strong intensity band at 2250 cm^{-1} and 1720 cm^{-1}. The compound shows only two singlets in the ratio of 3:2 in ^1H NMR spectrum. Identify the compound.	(A, CO 3)
2.	Predict the chemical shift values and spliting pattern in the proton NMR spectrum of 2-propylacetate.	(U, CO 1)
3.	Explain the resonance effect in IR absorption	(U)
4.	Calculate the λ_{max} of 2-dimethylidenecyclohexane	()
5.	Compare the $\pi \rightarrow \pi^*$ transitions of aniline and aniline in HCl.	()
6.	Predict the proton NMR spectrum of 2-methylpropanal	(U, CO 1)
7.	Pedict the chemical shift values of the olefinic protons in phenyl vinyl ether.	(U, CO 2)
8.	Explain overtones in IR spectrum.	(R, CO 1)
9.	Which ionisation method is most suitable for LC-MS. Rationalise your answer.	(A, CO 1)
10.	What are the possibe electronic aborption peaks in the UV spectrum of benzene?	()

(1 x 8 = 8)

PART B

Answer any 6 questions **Weights: 2**

11.	A compound ($C_6H_8O_2$) showed the following NMR data: Proton δ 2.0, 2.4, 2.5(t), 6.0(d), 7.0(doublet of triplet). Carbon-13 NMR δ 22, 24, 38, 130, 150, 199. Identify the structure and assign the data. Justify.	(A, CO 1, CO 3)
12.	Using Octant rule illustrate that axial haloketone rule is precursor of Octant rule.	()
13.	How can you distinguish between intermolecular H-bonding and Intramolecular H-bonding using IR Spectroscopy? Justify your answer.	(U, CO 1)
14.	An organic compound having molecular formula $C_8H_8O_2$ showed the following NMR data: Proton: δ 3.8, 6.9, 7.5, 7.75 and 10.4. Carbon-13: δ 55.5, 111, 120, 125, 128, 136, 161, 189. Identify the molecule, assign the data and predict the DEPT-135 and DEPT-90 spectra.	(A, CO 3)
15.	Write any five factors affecting the IR absorption. Explain how it is going to affect the vibrational frequencies	(U, CO 1)
16.	Propose a suitable structure of a molecule having a molecular ion peak at *m/z* 116 and another at 45 u. On MS/MS analysis, another peak at *m/z* 15 is also observed. Suggest any two prominent bands in the IR spectrum and assign them.	(An, CO 2)
17.	Mention any two application of ORD studies citing suitable examples.	()

18. An unknown substance shows a molecular ion peak at m/z 107 with relative intensity of 100. The M+1 peak has an intensity of 8. Propose a molecular formula. (An, CO 2)

(2 x 6 = 12)

PART C

Answer any 2 questions **Weights: 5**

19. A compound of molecular formula, $C_{16}H_{25}ON$ gave following spectral data: IR: 1690 (cm^{-1}); ^{1}H-NMR: 1.11 (t), 1.29 (d), 2.40 (q), 2.55 (t), 2.65 (t), 2.75 (m), 7.21 (d, J = 8Hz), 7.81 (d, J = 8Hz); ^{13}C NMR: 13.7, 24.2, 31.2, 38.8, 46.2, 47.5, 126.3, 128.5, 134.1, 152.5, 196.2; DEPT-135 spectrum shows five positive peaks and three negative peaks. MS (m/z): 247 (M+), 232, 218, 175, 161, 147. Find out structure of the compound and assign all the peaks. Sketch the COSY spectrum of the compound. (A)

20. An organic compound having molecular formula $C_8H_{14}O_2$ showed the following spectral data: Proton NMR δ 7.2, 6.1 (d, J=16Hz), 4.1, 2.7, 1.2, 1.0. Carbon-NMR: δ 170, 130, 119, 60, 30, 22, 14. DEPT 135 show 5 positive signals and one negative signal. IR spectrum showed absorption bands at (cm_{-1}) 1690, 2940, 1610. EI mass spectrum showed ions of m/z 142, 127, 97. Draw the predicted hetero cosy spectrum. (E, CO 3)

21. a) Briefly explain McLafferty rearrangement citing the example of three different types of compounds

b) The MS of an unknown organic compound shows M^+ peak at 87 (100%) and M+2 peak at m/z 89 (4.9%). It shows three signals in the ^{1}H NMR in the intensity ratio of 1:2:2 and strong absorption in IR at 3300-3500 cm^{-1}. Propose suitable structure to the compound. (A)

22. Write a note on ^{2}J and ^{3}J coupling interaction? Explain mechanism and the influence of various factors on the magnitude of coupling constant. In 4-allyloxyanisole, the -O-CH_2- protons comes to resonance at 1350.13, 1348.66, 1347.18, 1344.98, 1343.51 and 1342.04 Hz. Calculate the coupling constants. (U, CO 1)

(5 x 2 = 10)

OBE: Questions to Course Outcome Mapping

CO	Course Outcome Description	CL	Questions	Total Wt.
CO 1	Describe the principles of UV-visible, Chiro-optical, IR, NMR and Mass spectroscopic techniques.	U	2, 6, 8, 9, 11, 13, 15, 22	15
CO 2	Illustrate various spectroscopic techniques using simple problems.	An	7, 16, 18	5
CO 3	Elucidate the structure of an unknown organic compound using data from various spectroscopic techniques.	U	1, 11, 14, 20	10

Cognitive Level (CL): Cr - CREATE; E - EVALUATE; An - ANALYZE; A - APPLY; U - UNDERSTAND; R - REMEMBER;