Reg. No ....   Name **22P364**
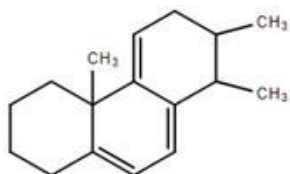
M. Sc. DEGREE END SEMESTER EXAMINATION : OCTOBER 2022
SEMESTER 3 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY
COURSE : **21P3CHET12 / 21P3CPHT12 : SPECTROSCOPIC METHODS IN CHEMISTRY**
(For Regular - 2021 Admission)

Duration : Three Hours   Max. Weights: 30

PART A
Answer any 8 questions   **Weight: 1**

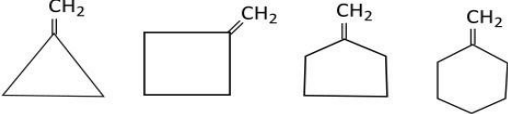|		
1.	What are NMR shift reagents ? Give an example	(U, CO 1)
2.	How can you differentiate between acetamide and acetic acid using IR spectroscopy?	(U, CO 1)
3.	Explain positive Cotton effect.	()
4.	An organic compound with molecular formula $C_4H_{10}O$ gives one triplet and one quartet in proton NMR spectrum (1.0 and 4.0). The carbon-13 NMR spectrum show only two signals, one is positive and other negative in DEPT-135 spectrum. Predict the structure of the compound.	(A, CO 3)
5.	Predict any two characteristic bands in the IR spectrum of formamide.	(U, CO 1)
6.	A structural isomer of C_7H_{14} shows seven signals in the noise decoupled ^{13}C NMR spectrum and only one negative signal in the DEPT-135 experiment. Identify the isomer.	(E, CO 3)
7.	Use the woodward rule to calculate λ_{max} for the compound	(U)

8.	How will you distinguish between methyl acetate and propanoic acid using NMR spectroscopy.	(U, CO 2)
9.	How will you distinguish between $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions? Apply the effect of solvation to illustrate this.	()
10.	An unknown substance shows a molecular ion peak at *m/z* 170 with relative intensity of 100. The M+1 peak has an intensity of 13.2 and M+2 peak has an intensity of 0.2. Propose a molecular formula.	(An, CO 2)

(1 x 8 = 8)

PART B
Answer any 6 questions   **Weights: 2**

11.	The HRMS mass of the molecular ion is 58.04185. This on dissociation gave an ion of *m/z*-15.02347. Propose a possible structure for the molecule and predict the important bands in the IR spectrum.	(A, CO 2)
12.	Discuss briefly on the stereochemical factors affecting the absoption maximum of organic compounds taking any two cases.	()
13.	Explain how to distinguish between the isomeric ketones of molecular formula $C_5H_{10}O$ using carbon-13 NMR spectroscopy.	(A, CO 2)

14. Predict the proton and carbon-13 NMR spectra of 2-nitropropane. Sketch the HMQC spectrum of the compound. (A, CO 2)

15. Arrange the following molecules in the increasing order of C = C stretching frequencies. Justify your answer. (A, CO 1)

16. On the basis of IR spectral data how will you differentiate between primary, secondary and tertiary amines? (A, CO 1)

17. 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)

18. Using Octant rule, predict the sign of the ORD curve of Trans-10-methyl-2-decalone. ()

(2 x 6 = 12)

PART C
Answer any 2 questions   Weights: 5

19. What is vicinal coupling ? Discuss AX, AX3, A2X2, A2X3 and AMX coupling systems taking one example for each. (U, CO 1)

20. Discuss in detail on Mc Lafferty Rearrangements citing atleast five different systems. (A, CO 1)

21. An organic compound with molecular formula $C_{10}H_{12}O_3$ showed the following spectra data: Proton NMR δ 1.4, 3.6, 4.0, 6.8, 7.2, 12.5. Carbon NMR δ 15, 40, 63, 115, 125, 130, 158, 179. DEPT-135 show positive signals for δ 15, 115, 130 and negative signals at δ 40 and 63. DEPT-90 show only two peaks δ 115 and 130. ^{1}H-^{1}H cosy show correlations (6.8-7.2) and (1.4-4.0). HMQC show correlations (1.4-15), (3.6-40), (4.0-63), (6.8-115), (7.2-130). EI mass spectrum showed ions of m/z 180, 135(100). IR spectrum shows a strong absorption band at 1720 cm^{-1}. Identify the structure and assign the data. (U, CO 3)

22. An organic compound having molecular formula $C_{11}H_{14}O_2$, showed the following spectral data: Proton NMR: δ 7.3, 5.1, 2.4, 1.1. Carbon NMR: δ 18, 34, 66, 135, 127, 128, 129, 178. DEPT-135 spectrum shows 5 positive signals and one negative signal. EI mass spectrum showed ions of m/z 178, 91, 71. IR 3060, 2940, 1730, 1200, identify the structure and explain the data. Sketch the predicted hetero cosy spectrum. (An, CO 3)

(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	1, 2, 5, 15, 16, 19, 20	17
CO 2	Illustrate various spectroscopic techniques using simple problems.	An	8, 10, 11, 13, 14, 17	10
CO 3	Elucidate the structure of an unknown organic compound using data from various spectroscopic techniques.	U	4, 6, 21, 22	12

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