Reg. No ..... Name **24P353**

MSc DEGREE END SEMESTER EXAMINATION- OCTOBER 2024

SEMESTER 3 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

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

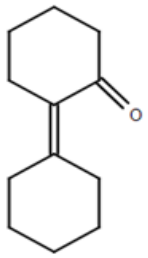
(For Regular 2023 Admission and Supplementary 2022/2021 Admissions)

Duration : Three Hours Max. Weights: 30

PART A

Answer any 8 questions **Weight: 1**

1. How can you differentiate between acetone and methylvinylketone using IR spectroscopy? (E, CO 1)
2. Predict the λ_{max} for an absorption band in the UV spetrum of the compound.



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3. Suggest any two fragment ions formed by the EI ionisation of cyclohexanone. (An, CO 2)
4. A 4-carbon compound showed two correlations in ^{1}H-^{1}H cosy and two correlations in ^{1}H-^{13}C cosy. There are two negative signals in DEPT-135. The EI mass spectrum showed ions of m/z 69.0578 and 43. Identify the structure. (U, CO 3)
5. How can *trans*-Cinnamic acid be differtiated from its cis- isomer using UV spectroscopy? ()
6. How will you distinguish between methyl acetate and propanoic acid using NMR spectroscopy. (U, CO 2)
7. How can IR- spectroscopy be used to distinguish 1-hexyne and 3-hexyne. Justify your answer. (E, CO 1)
8. Illustrate cis coupling and trans coupling using isomers dichloroethene as example (U, CO 1)
9. Explain hyperchromis shift with suitable examples. ()
10. The olefinic proton on the α-carbon has a higher chemical shift value than the protons on the β-carbon of methy vinyl ether. Why ? (A, CO 2)

(1 x 8 = 8)

PART B

Answer any 6 questions **Weights: 2**

11. Propose a suitable structure of a molecule having a molecular ion peak at *m/z* 115 and another at 44 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)
12. Does angle strain has any influence in the carbonyl streching frequency? Explain through an example (E)
13. *Meta*- tolualdehyde gave two intense peaks at m/z- 119 and 91 in its EI mass spectrum. Explain their formation. (An, CO 2)

14. Explain the factors affecting the chemical shift values of the protons in acetaldehyde and ethene (U, CO 1)

15. On the basis of IR spectral data how can you differentiate between primary, secondary and tertiary amides? (A, CO 1)

16. Explain the advantages of using an NMR instrument with higher field strength for recording the proton NMR spectrum. What will be the difference between the proton NMR spectrum of butyl bromide at 100 MHz and at 600 MHz ? (A, CO 2)

17. Discuss briefly on the stereochemical factors affecting the absoption maximum of organic compounds taking any two cases. ()

18. Using Octant rule, predict the sign of the ORD curve of Dihydrocarvone. ()

(2 x 6 = 12)

PART C

Answer any 2 questions **Weights: 5**

19. 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)

20. a) Briefly explain the electron impact ionization and desorption ionization methods
b) Outline the mode of fragmentation during mass spectrometric study of the following compounds leading to the peaks at indicated *m/z* (A, CO 1)
i) Methyl butanoate at m/z 74 and 59
ii) 2-Pentanone at m/z 71, 58 and 43

21. An organic compound (C_4H_8O) showed the following NMR data: Proton: δ 2.3(disappears on adding D_2O), 2.4, 3.6, 5.1, 5.8. Carbon: δ 37, 62, 117, 135. The DEPT-135 experiment showed one positive and three negative signals. Identify the molecule, explain the data, and sketch the possible Homo and hetero cosy spectra. (An, CO 1, CO 3)

22. Discuss Beckmann rearrangement and Benzoin condensation. Identify the reaction through spectoral analysis (A)

(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, 7, 8, 14, 15, 20, 21	17
CO 2	Illustrate various spectroscopic techniques using simple problems.	An	3, 6, 10, 11, 13, 16	9
CO 3	Elucidate the structure of an unknown organic compound using data from various spectroscopic techniques.	U	4, 19, 21	11

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