23144845

QP CODE: 23144845

Reg No : .....

Name : .....

M Sc DEGREE (CSS) EXAMINATION, NOVEMBER 2023

Third Semester

Faculty of Science

CORE - CH500303 - SPECTROSCOPIC METHODS IN CHEMISTRY

M Sc CHEMISTRY, M Sc ANALYTICAL CHEMISTRY, M Sc APPLIED CHEMISTRY , M Sc PHARMACEUTICAL CHEMISTRY, M Sc POLYMER CHEMISTRY

2019 ADMISSION ONWARDS

2D1109D2

Time: 3 Hours Weightage: 30

Part A (Short Answer Questions)

*Answer any **eight** questions.*

*Weight **1** each.*

1. How will you distinguish stereo isomers using ORD curves?
2. How will you estimate ring strain in IR spectra? Illustrate with an example.
3. Explain the presence of two C=O stretching frequencies in methyl ester of o-chloro benzoic acid.
4. Why Tetramethylsilane is used as the internal standard for calibrating chemical shift in NMR spectroscopy?
5. Why C-13 nuclei has Nuclear Magnetic Resonance while C-12 does not?
6. What is the splitting pattern in ABC and AMX type coupling?
7. Explain the term coupling constant. What is its unit?
8. Explain the following (a) Off resonance decoupling (b) lanthanide shift reagents.
9. Explain the strong peaks at m/e 91 and m/e 65 in Toluene.
10. Discuss the completion of pinacol-pinacolone rearrangement reaction using IR spectroscopy.

(8×1=8 weightage)

Part B (Short Essay/Problems)

*Answer any **six** questions.*

*Weight **2** each.*

11. Describe Woodward - Fieser rule for calculating λmax in dienes

12. A compound with molecular formula C3H6O can exist in two tautomeric forms A and B. The compounds shows prominent bands at (a) 1710cm-1 (b) 3250cm-1 and (c) 1630cm-1. Give the structure foe A and B for the above data.

13. Write a short note on NOE

14. Explain the principle and working of MRI technique.

15. An organic compound ($C_{13}H_{10}O$) showed the following NMR data: Proton: δ 7.45, 7.6, 7.8. Carbon-13: δ 128, 130, 132, 138 and 197. DEPT-90 showed three positive signals. Identify the molecule and assign the data.

16. Write briefly on MALDI and TOF in mass spectrometry.

17. Ethyl butanoate in its mass spectrum shows two characteristic peaks due to odd electron ions at m/z = 88 and 60 and an abundant ion at m/z = 71. Explain the fragmentation.

18. An organic compound with molecular formula $C_4H_8O_3$ gives the following spectral data. Deduce the structure.

    IR spectrum - 1705, 3410 cm^{-1}

    ^{1}H NMR - δ 4.15 (1H, sextet, J=7 Hz), 2.35 (2H, d, J=7Hz) and 1.2 (3H, d, J=7 Hz) ppm. Spectrum run in D_2O.

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

*Weight **5** each.*

19. *What is Cotton effect? Write down the applications. What is the importance of Cotton curves and plain curves.*

20. Briefly explain about 2D-NMR with Suitable example.

21. Write on the theory and applications of a) HRMS b) MSMS c) LC-MS d) GC-MS.

22. (a) A compound with molecular formula $C_4H_8O_3$ gave the following spectral data. Deduce the structure.

    IR: 1120, 1745 cm^{-1}

    ^{1}H NMR: δ 4.05 (2H, s), 3.8 (3H, s) and 3.5 (3H, s) ppm

    (b) Acetone reacts with two molar equivalents of benzaldehyde in presence of KOH and ethanol. Propose a structure for the product. The spectral data of the product are:

    ^{13}C NMR : δ 125, 128, 129, 130.5, 134.5, 144 and 185 ppm

    DEPT 135 –NIL

    DEPT 90 - δ 125, 128, 129, 130.5 and 144 ppm

    DEPT 45- δ 125, 128, 129, 130.5 and 144 ppm

(2×5=10 weightage)