R8268	Sub. Code
	536053

M.Sc. DEGREE EXAMINATION, APRIL – 2023

Fourth Semester

Chemistry

SPECTROSCOPIC METHODS OF ANALYSIS

(CBCS – 2019 onwards)

Time : 3 Hours Maximum : 75 Marks

Part A $(10 \times 2 = 20)$

Answer **all** the questions.

1. Define the Hook's equation.

2. Write the selection rules for Raman Spectra.

3. What is relationship between δ values (in ppm) and frequency (in Hz)?

4. Write an example of internal standards for NMR Spectra.

5. Define the hyperfine splitting.

6. The number of peaks in the ESR spectrum of CH_3 radical and $[C_6H_6]^-$ radical.

7. Calculate the expected apparent mass of the metastable ion produced when m/z 77 decomposes by loss of CH==CH to m/z 51?

8. Define even-electron rule.

9. Predict the structure of an organic compound with the following data:

Molecular formula: $C_5H_{11}Cl$; 1H NMR: δ 1.0 (t, 3H, 5.5 Hz), 1.5 (s, 6H), 1.8 (a, 2H, 5 Hz).

10. The 'H NMR spectrum of AX_3 exhibits lines at δ 2.1 and δ 2.3 ppm for X type proton and δ 4.1, 4.3, 4.5 and 4.7 ppm for A type proton from TMS at 100 MHz. What is the value of chemical shift (in ppm) A and X protons and coupling constant (in Hz)?

Part B $(5 \times 5 = 25)$

Answer **all** the questions, choosing either (a) or (b).

11. (a) Explain the theory of charge transfer complexes.

Or

(b) Explain the theory of surface enhanced Raman scattering (SERS) with example.

12. (a) Explain the factors influence the chemical shits in proton NMR.

Or

(b) Describe the applications of NMR in organometallic complexes with suitable examples.

13. (a) Explain the EPR spectrum of an octahedral V complex.

Or

(b) Explain the EPR spectra of hypothetical molecule H-X where X high spin complex of >1/2.

14. (a) Predict the masses of the ions produced in the mass spectrum of (i) 1-hexene and (ii) 2-heptene by the McLafferty rearrangement. Are these radical cations? What happens to the alkene fragments produced in these rearrangements?

Or

(b) Explain the significances of hyphenated techniques.

15. (a) The compound molecular formula: $C_8H_{10}O$; UV : 260 nm; IR : 3350, 3000-2900, 1610, 1580, 1450 cm^{-1}; 1H NMR : δ 1.30 (3H, d, 7 Hz), 4.9 (1H, q, 7 Hz), 7.3 (5H, bs), 2.8 (s, 1H, exchange with D_2O); 13 C NMR : 6 signals, CMR (SFORD) : one quartet, four doublets and one singlet. Mass: m/z 122, 107, 104, 77. Deduce the structure of compound.

Or

(b) Explain the principle and its importance of fluorescence spectroscopy.

Part C $(3 \times 10 = 30)$

Answer any **three** questions.

16. Explain the theory of mode of vibration and its factors influencing vibrational frequencies

17. Discuss the principles of spin-spin coupling and spin-spin splitting with examples.

18. (a) Describe the theory of zero-field splitting.

(b) Explain the ESR spectra of bis-salicyladimnecopper(II).

19. (a) Write a short note on principle and applications of MALDI-MS.

(b) Mass fragmentation of aliphatic and aromatic nitro compounds.

20. Explain the instrumentation of Mass spectra and EPR spectra with schematic diagrams.

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