



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – CHEMISTRY

FOURTH SEMESTER – APRIL 2017

CH 4809- APPLICATIONS OF SPECTROSCOPY

Date: 18-04-2017
Time: 09:00-12:00

Dept. No.

Max. : 100 Marks

Part-A

Answer ALL questions.

(10 × 2 = 20)

1. Why is the base peak formed at m/e 31 for methyl formate?
2. How will you distinguish among three isomeric butanols on the basis of mass spectrometry?
3. Why are the electronic absorption bands generally broad when compared to infra-red?
4. What is transannular conjugation? Give an example.
5. Why does 2,4,6-cycloheptatrienone show exceptionally low carbonyl stretching frequency?
6. Calculate the NMR frequency of proton in the field strength of 1.2 T. Given: $g_n = 5.5$.
7. Sketch the ^{31}P -NMR of H_3PO_2 .
8. Predict the number of ESR lines for tertiary butyl radical.
9. What is isomer shift?
10. Mention the significance of quadrupole coupling constant.

Part-B

Answer any EIGHT questions.

(8 × 5 = 40)

11. Explain the mass spectral pattern of cyclohexanone.
 12. What are charge transfer complexes? Explain their characteristics with an example.
 13. Discuss the fragmentation pattern of benzamide using mass spectrometry.
 14. Calculate λ_{max} of the following:
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15. Explain the structural determination of the molecule of the type XY_4 using IR and Raman spectroscopy.
 16. An organic compound with the molecular formula C_8H_6 decolorizes bromine in carbon tetrachloride and gives a white precipitate with ammonical silver nitrate solution. There is a sharp intense band at 3300 , 760 and 690 cm^{-1} and weak absorptions at 3085 and 2110 cm^{-1} . Also it shows broad and weak absorptions at 650 and 610 cm^{-1} . Identify the structure of the compound and explain.
 17. Explain the proton NMR spectra of HF and HCl molecules.
 18. Distinguish between homotopic and enantiotopic protons with examples.
 19. Discuss the isotropic and anisotropic nature of g values in molecules.
 20. Explain hyperfine coupling with an example.
 21. What are prolate and oblate nuclei? Give an example.
 22. While $\text{Fe}(\text{CO})_5$ shows quadrupole splitting, $\text{K}_4[\text{Fe}(\text{CN})_6]$ does not. Explain.

Part-C

Answer any **FOUR** questions.

(4 × 10 = 40)

23. An organic compound A (MF C₉H₁₀O₂) exhibits the following spectral data.
IR: 1745 cm⁻¹ (s), 1225 cm⁻¹ (broad, s), 749 cm⁻¹ (s) and 697 cm⁻¹ (s)
UV: λ_{max} at 268, 264, 262 and 257 nm
¹H NMR: δ 1.96 (3H,s), 5.00 (2H,s), 7.22 (5H,s)
Mass: m/e 91 (base peak)
Deduce the structure of the compound.
24. Draw and explain the Orgel energy level diagram of tetrahedral and octahedral complexes of Co²⁺.
- 25a. Explain the mass spectral pattern of hexanoic acid.
b. Distinguish between i) Maleic and fumaric acid and ii) propanaldehyde and acetone using IR spectroscopy. (5+5)
- 26a. Discuss the COSY of isopentyl methyl ketone.
b. Why is 'g' used as an index to interpret EPR spectra? (6+4)
- 27a. Predict the ¹⁹F- NMR of BrF₅ molecule and arrive at its structure.
b. Explain electric field gradient and quadrupole moment. (5+5)
- 28a. Discuss the Mossbauer spectrum of a nucleus with ground state spin 1/2 and excited state spin 3/2 when e²Qq ≠ 0; B = 0.
b. What are Kramer's doublets? Give an example. (6+4)
