

21P310

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Name:

Reg.No:

THIRD SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2022

(CBCSS - PG)

(Regular/Supplementary/Improvement)

CC19P CHE3 C09 - MOLECULAR SPECTROSCOPY

(Chemistry)

(2019 Admission onwards)

Time : 3 Hours

Maximum : 30 Weightage

Section A

Answer any *eight* questions. Each question carries 1 weightage.

1. Explain how microwave spectroscopy can be used for calculating the dipole moment of molecules.
2. What is zero field splitting? Explain with suitable example.
3. What is meant by first overtone?
4. Explain Fermi resonance.
5. Calculate the λ_{\max} of the following compounds.
6. Arrange the following compounds in the increasing order of vibrational frequency.
7. Discuss the utility of NMR spectroscopy in distinguishing enantiotopic and diastereotopic protons.
8. Expand INADEQUATE.
9. Give two examples for matrix used in MALDI.
10. What is hydrogen deficiency index? How is it useful?
11. What is meant by Stark effect?
12. In general IR absorption peaks of O-H group of phenols and alcohols are broad, why?

(8 × 1 = 8 Weightage)

Section B

Answer any *four* questions. Each question carries 3 weightage.

13. Explain g anisotropy and factors affecting g value.
14. Explain Frank-Condon principle for explaining the intensity of electronic transition.
15. How would you understand the electronic spectra of conjugated molecules using particle in a one dimensional box model? Discuss.
16. What is magnetic anisotropy effects in NMR spectroscopy?

17. Illustrate Nuclear Overhauser effect in NMR Spectroscopy using suitable example.
18. Demonstrate the mass spectra of 1-hexene and 2-hexene molecules. Identify molecular ion peak and base peak.
19. An organic compound with molecular formula C_4H_9NO gives the following spectral data. UV : λ_{max} 220nm. IR : 3500 (m), 3402 (m), 2960 (w), 1682 (s), 1610 (s). 1H NMR: δ 1.0 (doublet), 2.1 (septet), 8.1 (siglet). Determine the structure of the compound and explain the spectrum.

(4 × 3 = 12 Weightage)

Section C

Answer any *two* questions. Each question carries 5 weightage.

20. Discuss the factors affecting intensity and width of spectral lines.
21. Discuss (i) the classification of molecules on the basis of moment of inertia with examples (ii) Derive an expression for J_{max} for the rigid rotor at which there is maximum population.
22. (i) Explain spin-lattice relaxation method in NMR (ii) In the NMR spectrum of ^{14}N with $I = 1$, how many spectral lines will be observed. Calculate the frequency required for the NMR line at an external field of 1.4 T ($g_N = 0.403$, $\mu_N = 5.505 \times 10^{-27} \text{ JT}^{-1}$)
23. (a) Give a detailed account of methods to improve the sensitivity of ^{13}C nuclei in NMR spectroscopy.
(b) Explain the factors influencing the sensitivity of 1H and ^{13}C NMR spectroscopy.

(2 × 5 = 10 Weightage)
