

22P310

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Name: .....

Reg.No: .....

**THIRD SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2023**

(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. Which of the following molecules should have pure rotational spectra? (a) Deuterium, D<sub>2</sub> (b) HD (c) cis-1,2-Dichloroethylene (d) trans-1,2-Dichloroethylene (e) CHCl<sub>3</sub> (f) C<sub>60</sub>
2. How many ESR hyperfine lines are observed for p-nitro benzoate dianion molecule? Explain.
3. Explain the significance of the term 'gyromagnetic ratio'.
4. What are hot bands? Why are they called so?
5. Chloromethane has an absorption maximum at 172 nm, bromomethane shows an absorption at 204 nm, and iodomethane shows a band at 258nm. What type of transition is possible for each band? How can the trend of absorptions be explained?
6. How will you distinguish the following using IR spectroscopy? Nitro alkane and alkyl nitrites.
7. What is magnetic equivalence?
8. Do you think the axial and equatorial protons of cyclohexanes are chemical equivalent? Substantiate your answer.
9. Explain the relative intensity of isotopic peaks of the molecules containing Br
10. Illustrate retro-Diels-Alder fragmentation using a suitable example.
11. What is transition moment integral?
12. What are the common desorption ionization techniques employed in mass spectrometry?

**(8 × 1 = 8 Weightage)**

**Section B**

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

13. Define Stark effect. How it is useful for the calculation of Dipole moment of molecules?
14. Explain the classical theory of Raman effect

15. Write a short note on fingerprint region, fundamental frequency, first and second overtones and hotbands
16. arrange the following compounds in the increasing order of vibrational frequency and explain
17. Explain NOE in the context of  $^{13}\text{C}$  NMR. How is difference spectra utilised in distinguishing geometrical isomers?
18. Give an account of intensity enhancement of  $^{13}\text{C}$  NMR signal by polarization transfer technique.
19. Explain McLafferty rearrangement in mass spectra. Account for the  $m/z$  values 41, 42 and 43 in the mass spectra of 1-hexene

**(4 × 3 = 12 Weightage)**

### Section C

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

20. (i) Arrive at expressions for expression for rotational energy of a rigid diatomic molecule and symmetric top molecule (ii) Explain the effect of centrifugal distortion on the moment of inertia and energy of a diatomic molecule
21. Explain Mossbauer Effect. Explain the application of Mossbauer spectroscopy for the structural determination of iron complexes.
22. (i) State Frank - Condon principle. Discuss its importance in understanding the intensity of electronic transitions.  
(ii) Discuss the origin of P, Q, R lines in vibrational rotational spectrum of molecules.
23. (a) Discuss: Off-resonance and broad band decoupled spectra in NMR.  
(b) Integration of  $^{13}\text{C}$  NMR peaks does not give the quantitative information. Why?

**(2 × 5 = 10 Weightage)**

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