

23P310

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Name: .....

Reg.No: .....

**THIRD SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2024**

(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 the term Doppler Broadening.
2. Which of the following molecules should have pure rotational spectra? (a) Deuterium, D<sub>2</sub> (b) trans-1, 2-Dichloroethylene (c) CHCl<sub>3</sub> (d) C<sub>60</sub>
3. How many normal modes of vibrations are there for benzene molecule?
4. What is the use of Fortrat diagram in electronic spectroscopy?
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 intra and inter H bonding using IR spectroscopy?
7. Why is TMS used as reference molecule in NMR spectroscopy?
8. What is fluxionality? How is NMR used in its study?
9. Explain the relative intensity of isotopic peaks of the molecules containing Cl
10. What is rule of 13? Illustrate with an example.
11. Account for m/z= 65 in the mass spectrum of toluene.
12. How many ESR hyperfine lines are observed for CD<sub>3</sub> radical? Explain.

**(8 × 1 = 8 Weightage)**

**Section B**

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

13. Explain why NMR signal for protons in benzene is observed much downfield in comparison to that for protons in acetylene ?
14. Predict and explain whether UV/visible spectroscopy can be used to distinguish between the following pairs of compounds. If possible support your answers with calculations

15. Write a short note on fingerprint region, fundamental frequency, first and second overtones and hotbands
16. What are the salient features of a first order NMR spectrum? Is it possible to convert a non-first order spectrum to a first order NMR spectrum?
17. Integration of  $^{13}\text{C}$  NMR peaks does not give the quantitative information. Why?
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  $\text{C}_3\text{H}_9\text{N}$  shows the following peaks in the IR spectrum, 1)  $3012\text{ cm}^{-1}$  (m) 2)  $3425\text{ cm}^{-1}$  (s) 3)  $3236\text{ cm}^{-1}$  (m) 4)  $1615\text{ cm}^{-1}$  (m). When the compound A is treated with nitrous acid we get a compound B which shows a strong peak at  $3430\text{ cm}^{-1}$ . Identify A and B. Also explain the peaks in the IR spectrum.

**(4 × 3 = 12 Weightage)**

### Section C

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

20. Explain (i) Principle moments of inertia and classification of molecules based on that (ii) The polarisability ellipsoid for different vibrational modes of  $\text{CO}_2$  and sketch them.
21. (i) Discuss Kramers theorem with example (ii) Draw the energy level diagram and transitions for the  $\text{CD}_3$  radical and benzene anion (iii) Electron spin resonance is observed for atomic hydrogen with an instrument operating at 9.5 GHz. If the g value for the electron in the hydrogen atom is 2.0026, what is the magnetic field applied? ( $\mu\text{B}$ , Bohr magneton =  $9.274 \times 10^{-24}\text{ JT}^{-1}$ )
22. Explain the Classical and Quantum theory of Raman Effect.
23. (a) In a given organic compound two kinds of protons exhibit signals at 50Hz and at 200Hz using a 60MHz instrument. What will be their relative position using 400MHz instrument? Also convert the position of signals into delta scale.  
(b) Explain DEPT pulse sequence and working principle.

**(2 × 5 = 10 Weightage)**

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