

D 31104

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Name.....

Reg. No.....

**THIRD SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY)
EXAMINATION, NOVEMBER 2022**

(CBCSS)

Chemistry

CHE 3C 09—MOLECULAR SPECTROSCOPY

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 weightage

Section A

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

1. The rotation constant B and distortion constant D of a diatomic molecule are 10 and $4 \times 10^{-3} \text{ cm}^{-1}$ respectively. Find the frequency corresponding to J = 9 to J = 10 transition.
2. Explain with example overtones and combinations bands.
3. NO shows a Q branch in vibration-rotation spectrum. Why ?
4. Stokes lines are more intense than anti stokes lines in vibrational Raman spectrum. Why ?
5. Chemical shifts (δ) are field dependent but coupling constants J are field independent. Why ?
6. How many lines do you expect in the ESR spectrum of NH_3 radical ? Justify.
7. Predict λ_{max} for (a) 3-methyl pent-3-en-2-one ; (b) 
8. A set of protons absorb 180 Hz higher frequency w.r.t. TMS in a 100 MHz NMR spectrum. Calculate δ (delta) value.
9. Explain with example double resonance.
10. Explain FAB with reference to MS.

(8 \times 1 = 8 weightage)

Turn over

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Section B

*Answer any six questions.
Each question carries a weightage of 2.*

11. Discuss rotation spectra of symmetric top molecules.
12. The fundamental and first overtone of HCl are observed at 2886 and 5668 cm^{-1} respectively. Calculate the fundamental vibrational frequency and anharmonicity constant.
13. Briefly discuss a 2-dimensional NMR experiment.
14. Discuss isomershift in Mössbauer spectroscopy.
15. How would you establish configuration and conformation of cis and trans-decalones?
16. Distinguish chemical, magnetic and stereochemical equivalence in NMR.
17. What is DEPT with reference to NMR? Discuss.
18. Draw mass spectrum of butanone. Discuss.

$(6 \times 2 = 12 \text{ marks})$

Section C

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

19. State Franck Condon principle. Discuss its applications in understanding electronic transitions in diatomic molecules.
20. How do you achieve resonance condition in ESR spectroscopy? Discuss.
21. The spectral data of a compound is given:

IR 1740 cm^{-1} (s), 1160 cm^{-1} (s)

NMR 3.6δ (3H singlet), 1.2δ (9H singlet)

uv- no absorption

MS $\frac{m}{z}$ 116, 85, 59, 31

Deduce the structure and assign the peaks.

22. Discuss the theory, applications and instrumentation in Raman spectroscopy.

$(2 \times 5 = 10 \text{ marks})$