D 111107 **(Pages : 2)** **Name.....**

Reg. No.....

THIRD SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, NOVEMBER 2024

(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. Explain why NMR spectrum of benzene is observed at a lower field whereas that of acetylene is observed at higher field strength.
2. Which of the following molecules exhibit pure rotational spectra: HF, NH_3, CO_2, H_2O.
3. The force constant of $^{79}Br_2$ is 240 Nm^{-1}. Calculate the fundamental vibrational frequency and the zero point energy of $^{79}Br_2$.
4. What are the advantages of FT-NMR over the conventional NMR technique ?
5. Molecules possess only quantized energy levels and UV-Vis spectra are the result of electronic transitions. Still we observe a broad band in UV-V is spectroscopy. Explain.
6. Describe the effects of intramolecular and intermolecular hydrogen bonding on the position of IR absorption frequency of a compound. Give examples.
7. Explain the terms COSY and DEPT.
8. What is the effect of breakdown of Born-Oppenheimer approximation on P and R branches of the IR spectram of a diatomic molecule ?
9. What is g-factor in ESR ? State its significance.
10. Explain the importance of isotopic peak and base peak in mass spectra.

(8 × 1 = 8 weightage)

Turn over

Section B

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

11. Differentiate overtone and combination bands.

12. The rotational Raman spectrum $^{35}Cl_2$ shows a series of lines separated by 0.9752 cm^{-1} in both Stokes and anti-Stokes branches. Determine the bond length of Cl_2.

13. How is the dissociation energy of a diatomic molecule determined from the vibrational coarse structure in its electronic spectrum ?

14. Explain the rule of mutual exclusion and its converse. Sketch and explain the polarizability ellipsoids of the various modes of vibration of the CO_2 molecule. Which of these are Raman active ?

15. Explain the principle of ESR. Explain hyperfine coupling constant in ESR spectra.

16. Explain the isotope effect on the rotation spectrum.

17. Write a note on relaxation in NMR spectroscopy. Explain spin-lattice relaxation mechanism.

18. How do you distinguish primary and secondary alcohols by mass spectra ?

(6 × 2 = 12 weightage)

Section C

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

19. Explain the terms : i) FAB spectra ; ii) Cotton Effect ; iii) Mc Connell Relation ; iv) Woodward-Fieser rule.

20. Explain in detail various factors affecting the chemical shift in NMR.

21. a) Give an account of quantum theory in explaining Raman effect.

    b) Explain Stoke, antiStoke and Rayleigh phenomenon in Raman spectra.

22. a) Outline the principle of Mossbauer spectroscopy.

    b) Explain the applications of Mossbauer theory in the study of Fe(II) and Fe(III) cyanides.

(2 × 5 = 10 weightage)