LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

**M.Sc.** DEGREE EXAMINATION - **CHEMISTRY**

THIRD SEMESTER – NOVEMBER 2010

# CH 3810 - MOLECULAR SPECTROSCOPY

Date : 03-11-10 Dept. No. Max. : 100 Marks

Time : 9:00 - 12:00

Part – A

Answer **all** the questions (10 x 2 = 20)

1. Calculate the wavelength of a ball with 10 g mass and velocity , 2000 ms-1.
2. What do you mean by computer averaging enhancement of spectra?
3. What are Rayleigh ad Raman scattering?
4. Differentiate phosphorescence and fluorescence properties of excited molecules
5. What is photoelectric effect?
6. The NMR frequency of protons in a magnetic field intensity of 1T is 42.57 MHz.

Calculate the nuclear *g* factor for protons.

1. Vicinal coupling is minimum at 90º dihedral angle - why?
2. Sketch the EPR spectrum of •CD3 radical.
3. Mention the conditions to observe NQR transitions.
4. How will you obtain Mossbauer spectrum of a liquid sample?

Part – B

Answer any **EIGHT** questions (8 x 5 = 40)

1. Explain briefly the factors affecting the intensity of spectral transitions?
2. . Discuss the effect of isotopic substitution in the rotational spectrum of non rigid diatomic molecule.
3. Explain the principles of non-linear optical effects and frequency generation by them.
4. The exciting line is 5650 A0 and the Stokes line is 5800 A0. Calculate the wavelength of the anti-Stokes line.
5. Describe the vibrational spectrum of the anharmonic oscillating diatomic molecule
6. How does mutual exclusion principle help in resolving the geometry of chemical molecules?
7. How will you account for the positive and negative coupling constants in NMR?
8. How are the following identified in 2D NMR?
   1. non-adjacent groups
   2. long range coupling
9. EPR spectra are not presented as an absorption curve – Explain.
10. Explain the following
    1. asymmetric parameter in NQR
    2. pure NQR
11. Discuss the chemical ionization technique with suitable example.
12. Explain McLafferty rearrangement with an example.

# Part C

Answer any **FOUR** questions (4 x 10 = 40)

1. a) How are the rotational energy states determined by the magnitude of moment of

inertia for diatomic non-rigid rotor molecule? (5)

b) Calculate the rotational constant of HCl. The bond length is 136 cm-1. (5)

24. a) How are the vibrational energy states determined for simple harmonic diatomic

molecule? (5)

b)The bond length of ClF molecule is 0.1630 nm and the centrifugal distortion constant

is 10-4 B. Calculate the spacing between first eight lines. (5)

1. Explain the principles of Raman effects by i) Quantum theory ii) Classical theory.
2. a) What is a HETCOR spectrum? How will you interpret it? (6)

b) Distinguish between paramagnetic and diamagnetic anisotropy. (4)

27. a) Explain zero field splitting and hyperfine interaction in EPR with suitable examples. (6)

b) Draw an energy level diagram showing the ESR spectrum of an odd electron and compare it with the NMR spectrum of a bare proton. (4)

28.a) Explain isomer shift and quadupole splitting with relevant examples. (6)

b) How is X-axis is mass spectrum is calibrated in terms of m/e? What is the significance of molecular ion peak? (4)

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