



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION - CHEMISTRY

THIRD SEMESTER – NOVEMBER 2013

CH 3810 - MOLECULAR SPECTROSCOPY

Date : 09/11/2013

Dept. No.

Max. : 100 Marks

Time : 9:00 - 12:00

Part-A

Answer all questions. Each question carries two marks.

1. Calculate the force constant of C-C in alkane? The stretching frequency is 1280cm^{-1} .
2. What is a spherical top molecule? Give an example.
3. Mention the differences between Rayleigh and Raman Scattering.
4. State Frank Condon principle.
5. What are R-bands?
6. What is free induction decay?
7. Sketch the EPR spectrum of methyl radical.
8. If two signals differ by 1.5 ppm in a 60 MHz spectrometer, how do they differ in ppm in a 100 MHz spectrometer?
9. How many NQR transitions are possible for a nucleus of spin $I = 3/2$?
10. Mention the significance of quadrupole coupling constant.

Part-B

Answer eight questions. Each question carries five marks.

11. What are the factors affecting the width of the spectral lines? Explain.
12. Explain the types of transitions in electronic spectroscopy.
13. A particular molecule is known to undergo spectroscopic transitions between the ground state and two excited states, (a) and (b), its lifetime in (a) being about 10 s and in (b) about 0.1 s. Calculate the approximate uncertainty in the excited state energy levels and the widths of the associated spectral lines in hertz.
14. Explain the following for the linear and nonlinear polyatomic molecules.
(a) fundamental vibrations and (b) overtones and combination frequencies
15. Discuss the fingerprint absorption frequencies of functional groups for organic compounds in IR region.
16. The transmittance of an aqueous solution of KMnO_4 at a certain wavelength is 1 percent (0.01) or a 10^{-3} molar solution in a 1 cm cell. What is its absorbance and molar absorption coefficient?

17. Explain the calculation of coupling constant in ^1H NMR with an example.
18. Describe the splitting pattern observed in the low and high resolution ^1H NMR spectrum of propanaldehyde.
19. Sketch the EPR spectra of i) H_2^+ ii) D_2^+
20. What is pure NQR? Is pure NQR enough to calculate the quadrupole parameters in the case of ^{14}N containing compound?
21. While isomer shift is a function of S electron density, quadrupole splitting is not so – Explain.
22. Explain the fact that Mössbauer spectrum of $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$ shows two lines while that of $[\text{Fe}(\text{CN})_6]^{4-}$ shows only one line.

Part-C

Answer four questions. Each question carries ten marks.

23. Discuss the transition involved in the spectrum of a diatomic vibrating rotor with an example.
24. Draw Morse curve and explain the anharmonicity of the oscillator.
25. Assume the following data for the molecule $^1\text{H}^{35}\text{Cl}$:
 Bond length: 127.5 pm, Bond force constant : 516.3 n Nm^{-1} ,
 Atomic masses: $^1\text{H} = 1.60 \times 10^{-27}\text{ kg}$, $^{35}\text{Cl} = 58.06 \times 10^{-27}\text{ kg}$
 Calculate the following and give answers in cm^{-1}
 - (a) Zero point energy and the energy of fundamental vibration
 - (b) Rotational constant B
 - (c) Wave numbers of the lines $\text{P}_{(1)}$, $\text{P}_{(2)}$, $\text{P}_{(3)}$, $\text{R}_{(0)}$, $\text{R}_{(1)}$, $\text{R}_{(2)}$
26. (a) What is COSY? Discuss the COSY of n-propanol.
 (b) Explain geminal and vicinal coupling with examples (6+4)
27. (a) Explain isotropic and anisotropic hyperfine splitting with examples?
 (b) Why is EPR recorded in derivative mode? Justify the use of microwave radiation in EPR. (6+4)
28. (a) How is the oxidation state of an element determined the using Mossbauer spectroscopy?
 (b) What is asymmetry parameter? Mention its importance. (6+4)