 LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

THIRD SEMESTER – **NOVEMBER 2012**

# CH 3810 - MOLECULAR SPECTROSCOPY

Date : 06/11/2012 Dept. No. Max. : 100 Marks

Time : 9:00 - 12:00

**PART A**

Answer **all** the questions: 10x2=20

1. How are absorption and emission spectra formed?
2. Define S/N ratio.
3. Mention the differences between Rayleigh and Raman Scattering.
4. State Frank Condon principle.
5. How many normal modes of vibration are possible for HBr and SO2(bent) ?
6. Determine the magnetic field strength of an NMR instrument in which a proton chemical shift of 2.2ppm corresponds to a frequency of 1100Hz. Given gn = 5.585
7. Sketch the 1H NMR of pure n-propanol.
8. Obtain the ‘g’ value for Mn2+ complex.
9. Which of the following gives NQR? Chlorine liquid or Chlorine solid. Justify your choice.
10. When can a system exhibit quadrupole splitting?

**PART B**

Answer **any eight** questions: 8x5=40

11. What are the factors that affect the width of the spectral lines? Explain.

12. Explain the following for the linear and nonlinear polyatomic molecules.

a) fundamental vibrations b) overtones and combination frequencies

13. Briefly explain the principle of diatomic vibrating rotor when ΔJ = +1 and -1.

14. Discuss the different regions of the electromagnetic radiation.

15. Explain the fingerprint and absorption frequencies of functional groups for organic compounds in IR region?

16. Describe the effect of isotopic substitution in rotational spectra.

17. What are short range and long couplings? Give an example each.

18. Arrive at the structures of H3PO3 and H3PO2 whose 31P NMR show a doublet and a triplet respectively, when chemical exchange operates.

19. Explain isotropic and anisotropic hyperfine splitting with examples.

20. While isomershift is a function of S electron density, quadrupole splitting is not so – Explain.

21. What is pure NQR? Is pure NQR enough to calculate the quadrupole parameters in the case of 14N containing compound?

22. Sketch the EPR spectrum of i) H2+ ii) D2+

**PART C**

Answer **any four** questions: 4x10=40

23. Draw and explain Morse curve for an anharmonic oscillator.

24. Assume the following data for the molecule 1H35Cl:

Bond length:127.5pm, Bond force constant : 516.3Nm-1,

Atomic masses: 1H = 1.673x10-27kg, 35Cl = 58.06 x10-27kg

Calculate the following and give answers in cm-1

1. Zero point energy and the energy of fundamental vibration
2. Rotational constant B
3. Wave numbers of the lines P(1), P(2), P(3), R(0), R(1), R(2)

25. Discuss the principle of diatomic non-rigid rotor with an example.

26. a) The NQR frequencies for 2D in a compound are γ+ = 6 kHz and γ- = 5 kHz respectively. Calculate the asymmetry parameter η and the quadrupole coupling constant.

b) Explain the principle of FAB mass spectrometry.

27. a) Acetylenic protons are more shielded than ethylenic protons. – Justify.

b) What is COSY? Discuss the COSY of 1,3-dichloro propane.

28. a)How will you determine the oxidation state of an element using Mossbauer spectroscopy?

b) What is ‘g’ shift in EPR? How does it help to know the delocalization of

electron in a molecule?

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