 LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

THIRD SEMESTER – **APRIL 2012**

# CH 3810 - MOLECULAR SPECTROSCOPY

Date : 26-04-2012 Dept. No. Max. : 100 Marks

Time : 1:00 - 4:00

**PART – A**

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

1. Calculate the reduced mass and moment of inertia of D35Cl using internuclear distance of 0.1275nm.
2. Classify rotators into different kinds based on moment of inertia values.
3. What is the selection rule for Raman vibrational-rotational spectrum?
4. Wavelength of incident radiation is 5460 oA and Stokes line appear at 5520oA. Calculate the wavelength of anti Stoke line.
5. What is photoelectric effect? How does it help in explaining the principle of PES?
6. Calculate the strength of the magnetic field to get a precessional frequency of 100 MHz for 17O nucleus. Given: gn = 0.757.
7. Distinguish between diagonal and off-diagonal peaks in 2D NMR.
8. Account for the ‘zero’ asymmetry parameter observed in the case of axially symmetric molecules.
9. Define: Quadrupole splitting.
10. A free electron is placed in a magnetic field of strength 1.3T. If ge is 2.0023, and βe is 9.27x10-24 JT-1, find the ESR frequency in GHz.

**PART – B**

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

1. Explain the various factors affecting the intensity of spectral lines.
2. Write notes on i) chromophore and auxochrome ii) bathochromic and hypsochromic shift of UV band.
3. Describe Fermi resonance.
4. What is zero point energy? How does it explain the Raman scattering for molecules even when their vibrational quatum number is zero?
5. A microwave spectrometer capable of operating only between 60 and 90 cm-1 was used to observe rotational spectra of HI and DI.

HI (cm-1) DI (cm-1)

64.275 65.070

77.130 71.577

89.985 78.094

Find B, I, r for each molecule.

1. How does PES help in computing binding energy of electron in orbitals.
2. How is coupling constant calculated? Mention its significance.
3. Predict the spin-spin splitting patterns for 2,3-dimethyl butane and neopentane.
4. Explain i)zero field splitting ii) anisotropy in g value.
5. NQR spectroscopy lies between NMR and Mossbauer spectroscopy – explain.
6. The compound AB3 has C3 axis and its quadrupole resonance yields qzz a value of 3x1025. Find out its NQR frequency. Given: Q = -0.08x10-24cm2.
7. What is recoilless resonance emission and absorption? How can a Mossbauer nucleus be prevented from recoiling?

# PART-C

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

1. a) Derive the energy expression for anharmonic vibrator.

b) The fundamental, first and second overtones appear for HCl as 2886, 5668 and 8347cm-1 respectively. Calculate we and xe for HCl.

1. How do quantum theory and classical theory explain Ramaneffect?
2. How are IR and Raman spectroscopy helpful in explaining

i) SO2, as symmetric and bentii) CO2, as linear with center of symmetry

iii) N2O,linear without center of symmetry.

1. a) Explain i) Diamagnetic anisotropy ii) geminal and vicinal coupling

b) How are long range coupling detected in COSY?

1. a)Obtain the energy levels and show the NQR transitions possible in nucleus with spin i) I = 7/2 ii) I = 5/2.

b) Sketch the ESR spectrum possible for i) ˙NH2 radical ii) naphthalene in triplet state.

28.a) Discuss the Mossbauer transitions in 57Fe nucleus observed due to i) quadrupole splitting ii) hyperfine Zeeman splitting.

b)Explain the principle of FAB Mass spectrometry.

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