



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – PHYSICS

THIRD SEMESTER – NOVEMBER 2023

PPH3MC02 – SPECTROSCOPY

Date: 01-11-2023

Dept. No.

Max. : 100 Marks

Time: 01:00 PM - 04:00 PM

SECTION A – K1 (CO1)

Answer ALL the questions

(5 x 1 = 5)

1 Answer the following questions:

- a) The bond length of HF molecule is 0.0927 nm. calculate the moment of inertia of the HF molecule? (atomic masses: H = 1.673×10^{-27} kg; F = 31.55×10^{-27} kg)
- b) Explain Born – Oppenheimer approximation.
- c) Why Stokes lines are more intense than Anti-Stokes lines?
- d) A free electron is placed in a magnetic field of strength 1.5 T. Calculate the resonance frequency if $g = 2.0023$ and $\mu_B = 9.274 \times 10^{-24}$ JT⁻¹.
- e) What are spin-spin and spin-lattice relaxation processes?

SECTION A – K2 (CO1)

Answer ALL the questions

(5 x 1 = 5)

2 Choose the correct answer:

- a) Which is the correct reduced mass of HF?
(a) 5.72×10^{26} kg (b) 1.59×10^{-27} kg (c) 1.75×10^{-27} kg (d) 6.30×10^{26} kg
- b) Select the spherical top molecule from the following.
(a) CH₃F (b) H₂O (c) OCS (d) CH₄
- c) In Raman effect, an incident photon gains some energy from the atoms or molecules in a liquid and gets scattered. The scattered photon causes the spectral line of
(a) greater wavelength called Stokes' lines
(b) lesser wavelength called Stokes' lines
(c) greater wavelength called Antistokes' lines
(d) lesser wavelength called Antistokes' lines
- d) The range of electromagnetic radiation used in ESR spectroscopy is
(a) IR (b) UV (c) Visible (d) Microwave
- e) The spin quantum number, I of O¹⁷ nucleus is 5/2. The number of orientations of angular momentum vector, I of O¹⁷ nuclei in an external magnetic field is
(a) 11 (b) 6 (c) 7 (d) 10

SECTION B – K3 (CO2)

Answer any THREE of the following

(3 x 10 = 30)

- 3 (i) Explain the intensity variation in rotational spectrum and derive the expression for energy level J , with maximum population. (7)
- (ii) The average spacing between successive rotational lines of carbon monoxide molecule is 3.8626 cm^{-1} . Determine the transition which gives the most intense spectral line at temperature 300 K. (3)
- 4 Discuss about the fundamental vibrations of molecules and their symmetry.

5	State Franck-Condon Principle and explain its use in understanding the variation in the intensity of vibrational electronic spectra. (2+8)
6	Outline briefly each section of a Raman spectrometer using a neat schematic diagram.
7	Illustrate the interaction of nuclear spin with a magnetic field and deduce an expression for the energy associated with the transitions.
SECTION C – K4 (CO3)	
	Answer any TWO of the following (2 x 12.5 = 25)
8	(i) Outline the theory of rotational spectrum of a rigid diatomic molecule. (10) (ii) The separation between lines in the rotational spectrum of HCl molecule was found to be 20.92 cm^{-1} . Calculate the bond length. (atomic masses: $^1\text{H} = 1.673 \times 10^{-27} \text{ kg}$; $^{35}\text{Cl} = 58.06 \times 10^{-27} \text{ kg}$) (2.5)
9	Write a detailed note on dissociation energy and dissociation products.
10	Explain the theory of pure rotational Raman spectra of linear molecule.
11	Illustrate the vibration spectrum of a diatomic anharmonic oscillator.
SECTION D – K5 (CO4)	
	Answer any ONE of the following (1 x 15 = 15)
12	(i) What is chemical shift? Explain chemical shift and its measurement in NMR spectroscopy using methanol as an example. (2+10) (ii) An NMR signal for a compound is found to be 374 Hz downwards from TMS peak operating at 100 MHz. Calculate its chemical shift in p.p.m. (3)
13	Summarize the theory of Raman effect on the basis of classical and quantum theory.
SECTION E – K6 (CO5)	
	Answer any ONE of the following (1 x 20 = 20)
14	(i) Explain the impact of Doppler effect and uncertainty principle in obtaining Mossbauer spectrum. (ii) Calculate the recoil velocity of a free Mossbauer nucleus of mass $1.67 \times 10^{-25} \text{ kg}$ when emitting a γ -ray of 0.1 nm wavelength. What is the Doppler shift of the γ -ray frequency to an outside observer? (iii) With a block diagram, explain the working of Mossbauer spectrometer. (10+4+6)
15	Outline the influence of rotation on the vibration spectra of (i) Linear and (ii) Symmetric top molecules. (10+10)
