

M.Sc. CHEMISTRY
Second Semester (Repeat)
SPECTROSCOPY-I
(MSC – 204)

Duration: 3Hrs.

Full Marks: 70

Part-A (Objective) =20
Part-B (Descriptive) =50

(PART-B: Descriptive)

Duration: 2 hrs. 40 mins.

Marks: 50

Answer any four from Question no. 2 to 8
Question no. 1 is compulsory.

- (i) Deduce the expressions for the Stokes and anti Stokes Raman lines on the basis of Quantum theory. Explain the failure of classical theory and the success of Quantum theory over it. (3+2=5)

(ii) The rotational spectral lines of HCl molecule is separated by a distance of 20.8cm^{-1} . Calculate the bond length of the molecule. (5)
- (i) Deduce the relation showing the variation of intensity with path length. Define optical density and how is it related with transmittance? (3+1+1=5)

(ii) Write the rotational energy of a non rigid diatomic molecule. Mention the selection rule for transition. How the rotational energy and rotational spectra of non rigid diatomic molecule is different from rigid one? (2+1+1+1=5)
- (i) State the factors on which intensity of the spectral line depends. Explain the effects of those factors. (2+3=5)

(ii) Discuss how the intensity of rotational spectral lines changes with rotational Quantum number. Calculate the value of rotational quantum number (J) for maximum population. (2+3=5)

4. Why harmonic oscillator is not a true model of a vibrating diatomic molecule? How can you convert a harmonic oscillator to an anharmonic oscillator? Write down the energy of the anharmonic oscillator. Deduce the frequencies of fundamental, first overtone, second overtone and first hot band. Draw the potential energy versus displacement curve of an anharmonic oscillator. (2+1+2+4+1=10)
5. (i) Explain the symmetry properties of rotational energy levels of a diatomic molecule and the effect of nuclear spin on it. (5)
- (ii) Write down the rotational energy of a symmetric top molecule and deduce the frequency of transition stating the selection rule. (2+2+1=5)
6. (i) Define chemical shift and explain the origin of it taking CH_3OH as an example. (1+4=5)
- (ii) Discuss the principle of proton NMR spectroscopy and deduce the condition of resonance. (4+1=5)
7. (i) Calculate the frequencies of P, Q and R branches of rotational spectral lines in vibrational transitions. Mention the selection rules. (3+2=5)
- (ii) Calculate the magnetic field for a 500 MHz proton NMR spectrometer. Given that ($\beta_N = 5.05 \times 10^{-27} \text{ J T}^{-1}$, $g = 5.585$ and $h = 6.63 \times 10^{-34} \text{ J.S}$). (2)
- (iii) Discuss the rotational Raman spectra of $^{16}\text{O}_2$. (3)
8. (i) Explain what do you mean by spin-spin coupling? Discuss the high resolution NMR spectra of dry and pure ethanol. (2+3=5)
- (ii) What are different types of relaxation in NMR spectroscopy? Explain. How relaxation is related with the breadth of NMR signal? (2+2+1=5)
