7. (a) Using an appropriate energy level diagram and selection rules show the magnetic hyperfine structure in the Mossbauer spectrum of a nucleus with ground state and excited state spins equal to 3/2 and 5/2, respectively. Show the spectral transitions and the appearance of the spectrum.

(b) Explain with examples the isomer shift in MB spectroscopy.

(c) What are essential conditions to be observed to obtain Mossbauer spectrum ? Explain how the tuning is achieved experimentally.

(d) "Low and high spin complexes can be distinguished by Mossbauer spectroscopy." Explain the statement.

8. (a) How can $^{14}N(I = 1)$, NQR spectroscopic studies be used to determine the structure of BrCN ?

(b) How would you get information about the structure of a compound from its NQR data ? Explain taking an example.

(c) Explain the effect of crystal lattice on the magnitude of eQq data in NQR spectroscopy.

(d) Discuss the relationship between electric field gradient and the molecular structure in concern of NQR spectroscopy.

Exam. Code : 210402
Subject Code : 4951

M.Sc. Chemistry 2nd Semester

SPECTROSCOPY B : TECHNIQUES FOR STRUCTURE ELUCIDATION OF INORGANIC COMPOUNDS

Course—XII

Time Allowed—2 Hours] [Maximum Marks—75

Note :— There are ***eight*** questions of equal marks. Candidates are required to attempt any ***four*** questions.

1. (a) Describe the factors on which the relative intensities of the rotational spectral lines depend.

(b) How do overtones, combination bands and fermi resonance arise in the IR spectrum ?

(c) The fundamental and first overtone frequencies of $^{14}N^{16}O$ are centered at 1876 cm^{-1} and 3724 cm^{-1} respectively. Evaluate the equilibrium vibrational frequency, the anharmonicity, exact zero point energy and the force constant of the molecule ? Explain the pure rotational Raman spectrum for a linear diatomic molecule.

2. (a) What is meant by Raman and Rayleigh scattering ? Discuss the Quantum Mechanical theory of Raman spectroscopy.

(b) Draw and explain a schematic diagram of the vibrational rotation Raman spectrum of a gaseous diatomic molecule.

(c) Calculate the relative Boltzmann population at 127ºC of :

(i) The first two IR energy levels separated by 2000 cm^{-1}

(ii) The first two electronic energy levels separated by 120 kJ mol^{-1}

(d) Discuss rule of mutual exclusion and finger printing in concern of spectroscopic studies.

3. (a) Can IR and Raman spectroscopic studies be useful to differentiate between *cis* and *trans* isomers of $[Co(bipy)_2Cl_2]Cl$? Explain.

(b) Define symmetry and explain about five symmetry elements taking suitable examples of molecules.

(c) Determine the point group of the following molecules :

(i) K_2PtCl_4

(ii) trans $[Pt(NH_3)_2Cl_2]$

(iii) CO_3^{2-}

(iv) NO_3^-

(v) H_2S.

4. (a) How does IR spectroscopy determine the mode of coordination of NO_3^- and CO_3^{2-} ions ?

(b) Explain how IR spectroscopy is used in structure elucidation of metal carbonyls.

(c) How is IR spectroscopy applied to distinguish between lattice and coordinated water ?

(d) Does metal-coordinated N, N-dimethylacetamide show any change in carbonyl absorption ? Give reason.

5. (a) Photoelectrons ejected from O_2 using He-I radiation (wave length 584 Å) have kinetic energies of 5.82 Ev. Calculate the ionisation energy of O_2 molecule.

(b) Give a detailed note on core level photoelectron spectroscopy.

(c) How the chemical environment of the atoms effect the core electron binding energies in photoelectron spectrum ? Explain taking suitable example.

(d) Explain the effect of spin-orbit coupling on photoelectron spectra of noble gases.

6. (a) Discuss principle and applications of ELDOR spectroscopy.

(b) Explain why the ESR spectrum of an unpaired electron interacting with two equivalent protons shows three lines with intensity 1:2:1.

(c) Discuss the ESR spectrum and hyperfine splitting in :

(i) Radical anion of Pyrazine

(ii) 1,4-benzosemiquinone anion.

(d) Explain the double resonance in ESR spectroscopy.