PG – 815

II Semester M.Sc. Examination, June 2015
(NS) (2010-11 and Onwards)
CHEMISTRY
C – 204 : Spectroscopy – I

Time : 3 Hours Max. Marks : 80

Instruction *: Answer question No.* ***1*** *and* ***any five*** *of the remaining.*

1. Answer **any ten** of the following : **(10×2=20)**

   a) How many operations are generated by S_5-axis ? Write each in a systematic way.

   b) What are the symmetry elements and operations associated with a planar AB_3 molecule ?

   c) Show that the conjugate matrices have identical characters.

   d) A non-linear triatomic molecule has nine degrees of freedom. How many stretching and bending modes are present in it ?

   e) Microwave spectra are difficult to be observed in solids and liquids. Why ?

   f) Explain fermi resonance by taking CO_2 molecule as an example.

   g) Symmetric top molecules have polarizability ellipsoids whereas spherical top molecules have spherical polarizability surfaces. Account for this.

   h) State the terms fluorescence and phosphorescence using a sketch of the energy diagram.

   i) Distinguish between parallel and perpendicular bands. Give an example for each.

   j) How many irreducible representations are present in C_{2h}-point group ? Justify your answer.

   k) The odd-even classification of orbitals does not arise in heteronuclear diatomic molecules. Why ?

   l) How are σ_- and π_- molecular orbitals obtained ?

2. a) Construct the character table for C_{3v} - point group, stating the rules employed stepwise in the process and assign the Mulliken symbols.

   b) Using the above character table, deduce the transformation of the normal modes of vibration of ammonia molecule into irreducible representations. **(6+6=12)**

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3. a) The rotational spectrum of CO shows a series of lines spaced 3.8424 cm^{-1} apart. Calculate the moment of inertia and bond length of C = 0 bond.

   b) Draw a schematic diagram of microwave spectrometer and mention the function of its components.

   c) Derive the Orthonormalization conditions of wave functions based on symmetry concept. **(3+4+5=12)**

4. a) In polyatomic molecules, the actual number of modes of vibrations will be different from those calculated theoretically. Explain.

   b) State and explain the selection rules for electronic transitions.

   c) How does the breakdown of the Born-Oppenheimer approximation affect the P and R branch lines of the vibration rotation spectrum of a diatomic molecule ? **(3+4+5=12)**

5. a) Discuss the classical theory of Raman effect.

   b) Draw the orbital pictures for an AH_2 molecule and show the change in energy of the various orbitals as the bond angle changes from 90° to 180°. **(6+6=12)**

6. a) Depict the energy level diagram and show how the energy of the 1s σ_g and 1s σ_u^* orbitals varies with the distance between the nuclei.

   b) Discuss briefly on non-radiative decay processes. **(6+6=12)**

7. a) Write a short note on Fortrat Parabolae.

   b) Give the selection rules for IR and Raman Spectroscopy.

   c) Draw a schematic diagram of Michelson interferometer and discuss the experimental technique and list the advantages of FT technique. **(3+3+6=12)**