CURRICULUM

HEMCHANDRACHARYA

NORTH GUJARAT UNIVERSITY, PATAN

M.Sc. (Chemistry) Semester - 1

Course:CHNN–404(Corecompulsory)

Symmetry, Group Theory & Spectroscopy

UNIT-01 Symmetry & Group Theory

16 Hrs

- Outline of symmetry elements and symmetry operation
- Schonflies method for determining the point group of the molecules.
- Multiplication of symmetry operation and multiplication table for C_2v, C_3v, C_{2h}.
- Equivalent symmetry elements, similarity transformation and conjugacy of symmetry operation within the point group
- Matrics: Characteristics,types of matrices(common & special),and Algebra of matrices(Particularly Multiplication)
  Use of Matrix and matrix representation of symmetryElements and Their point groups(using variousVectors: position vector, translation vector, base vector)
- Γ_{3N} Representation :For H_2O,NH_3,BF_3,$PtCl_4$,PCl_5,SF_6,$POCl_3$,CCl_4,Cis &Trans N_2F_4, $XeOF_4$
- Reducible and Irreducible Representation& charactor Table
- Characteristics of Irreducible Representation: The great orthogonality theorem
- Construction of Character Table For C_3v using properties of irreducible Representation
- Direct product and its utility.

UNIT 02 : Group theory and its applications

16 Hrs

- Character table and their presentation
- Reduction formula for reducible representation of any matrix presentation of particular point groups
- Application of symmetry to hybrid orbital, molecular orbital
- Hybridisation schemes for sigma-orbitals (for AB_3 : planar triangle, trigonal pyramidal e.g. BF_3 & NH_3 , AB_4 : tetrahedral and square planar molecules e.g. CH_4& $[PtCl_4]^{-2}$, AB_5 : trigonal bipyramidal & square pyramidal e.g. PCl_5 & IF_5 and AB_6 : octahedral e.g. SF_6 and pi-orbital for AB_3 (e.g. BF_3) AB_6 (e.g. SF_6)
- Application of symmetry to molecular vibrations, interpretation of IR & Raman activity. (spectral data)

15.

UNIT 03 : Unifying principles of spectroscopy. **15 Hrs**

Electromagnetic radiation, interaction of electromagnetic radiation with matter absorption,emission,transmission,reflection,refraction,polarisation and scattering, Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory ,transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels.

UNIT 04 : Mossbauer spectroscopy **13 Hrs**

- Introduction
- Interpretation of isomer shifts
- Quadruped interactions
- Paramagnetic Mossbauer Spectra
- Mossbauer Emission Spectroscopy
- Application 5