Course No: PGCHM17E105

Title: Symmetry and Group Theory (02 Credits)

Max. Marks: 50 ***Duration: 32 Contact hours***

Continuous Assessment: 10 *End Term Assessment: 40*

Unit-I Molecular Symmetry (16 Contact hours)

Molecular Symmetry - Symmetry elements and operations: Identity, rotation axis, reflection plane, inversion centre, improper rotation axis. Combination of symmetry operations, Symmetry groups and group multiplication tables.

Symmetry Classification of molecules: Point groups. Schoenflies notation of point groups. Identification of point groups. Matrices and their combination, block factored matrices, Matrix representation of symmetry operations.

Unit-II Character Tables and Spectroscopy (16 Contact hours)

The Great Orthoganality Theorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations, Mullikan symbols for IRS. Character table-construction of character tables for C2v, C3v and C4v point groups. Applications of group theory to IR and Raman spectroscopy, Symmetry of IR and Raman active normal vibrational modes of AB2, AB3, AB4, AB5, and AB6 type molecules. Applications of symmetry to Molecular Chirality and Polarity.

Books Recommended

1. Chemical Applications of Group Theory; 2nd edn.; F.A.Cotton; Wiley Eastern; 1994)
2. Molecular Symmetry and Group Theory; L. Carter; Wiley; 1998.
3. Symmetry and Spectroscopy of Molecules; K. Veera Reddy; New Age 1998.
4. Inorganic Chemistry, Principles of structure and reactivity; 4th Edition; James E. Huheey, Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc.

Course No: PGCHM17E106

Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: 50 ***Duration: 32 Contact hours***

Continuous Assessment: 10 *End Term Assessment: 40*

Unit-I

(a) Fundamentals of Spectroscopy (08 Contact hours)

Interaction of light with matter, transition probability, transition moment integral, derivation of selection rules. Intensity of spectral lines; Einstein's treatment of absorption and emission processes. Beer Lambert Law: Transmittance, Absorbance, Molar Integrated Intensity, Oscillator strength. Natural spectral line width, broadening of spectral lines -Doppler and Collision effects.

(b)Electronic and Photoelectron Spectroscopy (08 Contact hours)

Electronic Spectroscopy: Vibronic transitions. Intensity of spectra, the Franck-Condon principle. Electronic spectra of organic molecules, chromophores, auxochrome, and spectral shifts Different types of electronic transitions; nomenclature, symmetry labels of electronic states--spectra of formaldehyde, Symmetry selection rules, Term Symbol (Elementary Idea). Effects of solvent, electron withdrawing and electron donating groups, conjugation and extended conjugation on the position of spectral bands. ***Photoelectron Spectroscopy:*** Basic principles- photoionization process; ionization energies; Koopman's theorem. Photoelectron spectra of simple molecules (N2, O2),

Unit-II

(a) Infrared Spectroscopy (08 Contact hours)

Linear harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, Morse potential energy levels. Fundamental bands, overtones and hot bands. Vibration- rotation spectra of diatomic molecules; P, Q and R branches; Vibrations of polyatomic molecules: Normal vibrational modes, selection rules; combination and difference bands. Factors influencing the band positions and intensities. Group frequencies and finger print region.

(b)Raman Spectroscopy **(08 Contact hours)**

Classical and Quantum theories of Raman scattering, Molecular polarizability, rotational, vibrational, and vibrational-rotational Raman spectra. Selection rules; rule of mutual exclusion. Applications.

Books Recommended

1. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.\
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.