DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : **IV (Code-MCH-404)**
Compulsory / Optional : **Compulsory**
Max. Marks : **100**

Paper – IV : Group Theory & Spectroscopy I

Unit – I	**Symmetry and Group theory in Chemistry** Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schonfilies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} group to be worked out explicity). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group Symmetry aspects of molecular vibrations of H_2O molecule.
Unit – II	**Microwave Spectroscopy** Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.
Unit – III	**Infrared Spectroscopy** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations, normal co-ordinate analysis.
Unit – IV	**Raman Spectroscopy** Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent anti stokes Raman spectroscopy (CARS).
Unit –V	**Electronic Spectroscopy** **Molecular Spectroscopy** Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra. **Photoelectron Spectroscopy** Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy-basic idea.

oks suggested:

1. Modern Spectroscopy, J.M. Hollas, John Viley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH- Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.