MC-04

GROUP THEORY, SPECTROSCOPY AND DIFFRACTION METHOD

(Question will be set from each unit/section with internal choice)

Marks - 100 | 90 Hrs. (3 Hrs./Week)

Units	Topics
I	**Symmetry and Group Theory in Chemistry** — 12 Hrs Symmetry elements and symmetry operation, definition of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. **Unifying Principles** — 10 Hrs. Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, 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.
II	**Microwave Spectroscopy** — 3 Hrs. 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. **Vibrational Spectroscopy** — 12 Hrs. A. **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. B. **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 spectroscopoy (CARS).
III	**Electronic Spectroscopy** — 12 Hrs. A. **Atomic Spectroscopy:** Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms. B. **Molecular Spectroscopy:** Energy levels, molecular orbitals, vibronic transitions, vibrational progression and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra. C. **Photoelectron Spectroscopy:** Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Anger electron spectroscopy basic idea. **Photoacoustic Spectroscopy** — 3 Hrs. Basic principles of photoacoustic spectroscopy (PAS), PAS-gases and

condensed systems, chemical and surface applications.

IV **Magnetic Resonance Spectroscopy** **20 Hrs.**

A. **Nuclear Magnetic Resonance Spectroscopy:** Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J', Classification (ABX, AMX, ABC, A_2B_2 etc.) spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton - 13_C, 19_F and 31_P, FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

B. **Electron Spin Resonance Spectroscopy:** Basic principles, zero field splitting and kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnel relationship, measurement techniques, applications.

C. **Nuclear Quandrupole Resonance Spectroscopy:** Quadrupole nuclei, quadrupole moments, electric field gradient, copuling constant, splittings. Applications.

V **X-ray Diffraction** **12 Hrs.**

Bragg condition, Miler indices, laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

Electron Diffraction **3 Hrs.**

Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron Diffraction **3 Hrs.**

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.