Paper-IV CHN-404 A
Group Theory, Spectroscopy and Diffraction Methods

I Symmetry and Group Theory in Chemistry 9 Hrs

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schönflies 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.

II Unifying Principles 7 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.

III X-ray Diffraction 8 Hrs

Bragg condition, Miller 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.

IV Moss Bauer Spectroscopy 7 Hrs

- Introduction
- Interpretation of isomer shifts
- Quadrupde interactions
- Paramagnetic Mossbauer Spectra
- Mossbauer Emission Spectroscopy
- Applications