M. Sc. II Sem

MCH – 204: Spectroscopy II and Diffraction Methods

Unit – I

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 (AXB, AMX, ABC, A2B2 etc) spin decoupling; basic ideas about instrument, NMR studies of nuclei other then proton-^{13}C, ^{19}F and ^{31}P FT NMR, advantages of FT NMR.

Unit – II

Electron Spin Resonance Spectroscopy :

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value, lsotropic and anisotropic hyperfine coupling constants, spin Hamiltonian. Spin densities and McConnell relationship, measurement techniques, applications.

Unit-III

X-ray Diffraction-I

Generation of X-rays, X-ray tubes, Synchrotron source, Lattice, planes, Miller indices, X-ray diffraction, Bragg's law, Reciprocal lattice, Crystal symmetry, space groups, Systematic absences, Crystal growing, screening and mounting, Data

collection, Data reduction, Theory of Structure factors and Fourier Syntheses, Phase problem and its solution, Structure solution and refinement.

Unit-IV

X-ray Diffraction-II

Derivation of X-ray results, Determination of absolute configuration of the molecules, Overview of important crystallographic programmes, Random and Systematic errors, File structure for SHELXL and its commands, Diagrams, Tables, Use of XP, Structure Validation, Disorder, Types of disorder and their solution, solvent disorder, Twining, Types of twining and their solution. Crystallographic database.

Unit – V

Electron Diffraction :

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 :

Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cells.

Books 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, McGraw Hill.
7. Basic Principles of Spectroscopy, R. Chang, McGraw 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.