SEMESTER-III
Paper-S-3041
Advanced Spectroscopic Techniques

Time: 3 Hrs. **M.M. 75 marks**
Note: The paper will be divided into two sections.

Section-A One question with 10 parts (short answer word limit 20) spread over whole syllabus. Each part will be of 1 mark and candidate is required to attempt all the ten parts

Total 10 marks

Section-B Five questions (answer not exceeding 500 words) are from each Unit with internal choice will be asked and the candidate is required to attempt all five questions. Each question will be of 13 marks **Total 65 marks**

UNIT-I

Mass Spectrometry: Introduction, ion production - El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement.Retro Diel -Alder reaction, Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

UNIT II

Nuclear Magnetic Resonance Spectroscopy: General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra-nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-^{19}F, ^{31}P.

Carbon-13 NMR Spectroscopy General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.

Two dimension NMR Spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

UNIT III

Electron Spin Resonance Spectroscopy: Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and inorganic free radicals such as PH_4, F_2 and $[BH_3]$.

UNIT IV

X-ray Diffraction: 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.

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 and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

UNIT V

Mössbauer Spectroscopy: Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds - nature of M-L bond, -coordination number, structure (3) detection of oxidation state and equivalent MB atoms

Books Suggested

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry edi R.L. Carlin vol. 3, Dekker
6. Inorganic Electronic Spectroscopy,. A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Norwood.
8. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J. Martin, Heyden.
9. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley
10. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
11. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
12. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill.
13. Modern Spectroscopy, J.M. Hollas, John Wiley.
14. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
15. NMR, NQR, EPR and Msssbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
16. Physical Methods in Chemistry, R.S. Drago, Saunders College.
17. Chemical Applications of Group Theory, F. A. Cotton.
18. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
19. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
20. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.

21. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
22. Introduction to Magnetic Resonance, A Carrington and A.D. Maclachalan, Harper & Row.