SLIET LONGOWAL

2.4.7 - CHEMISTRY (Ph.D. - CHY)

Course work Subject codes and subject names

SUB CODE	SUBJECT NAME
AC-10801	ADVANCED SPECTROSCOPIC TECHNIQUES
AC-10802	NEWER METHODS IN ORGANIC SYNTHESIS
AC-10803	ADVANCES IN ENVIRONMENTAL CHEMISTRY
AC-10804	COMPUTATIONAL CHEMISTRY
AC-10805	SUPRAMOLECULAR CHEMISTRY

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AC 10801 ADVANCED SPECTROSCOPIC TECHNIQUES

Ultraviolet and Visible Spectroscopy: Various electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic heterocyclic compounds, organometallic compounds, coordination and charge transfer complexes.

Infrared Spectroscopy: Instrumentation and sample handling. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids, inorganic and organic compounds.

Nuclear Magnetic Resonance Spectroscopy: General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, 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 curvevariation of coupling constant with dihedral angle. Simplification of complex spectranuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F & P. Two dimension NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Application of nmr spectroscopy to paramagnetic substances. Carbon-13 NMR Spectroscopy**:** General considerations, chemical shift, coupling constants.

Mass Spectrometry: Introduction, ion production - EI, CI, 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. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

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 McConnell relationship, measurement techniques, applications.

References:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
3. Progress in Inorganic Chemistry vol., 8, ed., FA Cotton, vol., 15, ed. S.J. Lippard, Wiley.
4. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
5. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
6. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J. Mirtin, Heyden.

7. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.
8. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
9. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
10. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill.

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AC 10802 NEWER METHODS IN ORGANIC SYNTHESIS

Green Synthesis Principles: Prevention of Waste/By-Products, Maximum Incorporation of the Reactants into the Final Product, Prevention or Minimization of Hazardous Products, Designing Safer Chemicals, Energy Requirements for Synthesis, Selection of Appropriate Solvent, Selection of Starting Materials, Use of Protecting Groups, Use of Catalyst, Strengthening of Analytical Techniques.

Phase Transfer Catalysis: Introduction, Applications of PTC in Organic Synthesis, Oxidation Using Hydrogen Peroxide Under PTC Condition, Crown Ethers.

Microwave Induced Synthesis: Introduction, Applications - Microwave Assisted Reactions in Water, Microwave Assisted Reactions in Organic Solvents, Microwave Solvent Free Reactions (Solid State Reactions). Solid Supported Organic Synthesis.

Ultrasound Assisted Synthesis: Introduction, Applications of Ultrasound in organic synthesis. Solid Supported Organic Synthesis.

Aqueous Phase Reactions: Introduction, Diels-Alder Reaction, Claisen Rearrangement, Wittig-Homer Reaction, Michael Reaction, Aldol Condensation, Knoevenagel Reaction, Pinacol Coupling, Benzoin Condensation, Claisen- Schmidt Condensation, Heck Reaction, Strecker Synthesis, Wurtz Reaction, Oxidations, Reductions, Polymerisation Reactions, Photochemical Reactions, Electrochemical Synthesis, Miscellaneous Reactions in Aqueous Phase.

Ionic Liquids: Green Solvents, Reactions in acidic Ionic Liquids, Reactions in Neutral Ionic Liquids.

References:

1. Latest references (Reviews/Books) on the above topics.

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AC 10803 ADVANCES IN ENVIRONMENTAL CHEMISTRY

AtmospherIC Photochemistry: Chemical composition of atmosphere - particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere. Principal of photochemistry, Kinetics of photochemical processes, Reactions in the upper atmosphere, Photo-processes in the troposphere, Photochemical smog, Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Hydrosphere: Water in the Environment, Water quality standards. Acid-base properties, Oxidation-reduction processes, complexation in natural systems, Adsorption and ion-exchange processes, Purification and treatment of water. Analytical methods for measuring BOD, DO, COD, F, Oils, residual chloride and chlorine demand.

Halo-organics and Pesticides: Chemistry of haloorganics: synthesis, reaction, microbial degradation and toxicity. Herbisides and organo-phosphorous insecticides: synthesis, reaction, environmental degradation and toxicity; Proposed phase out of all chlorine containing compounds.

Environmental Toxicology: Chemical solutions to environmental problems, biodegradability, Bioremediation of the environmental pollutants.

Emerging pollutants in the environment: Nanoparticles, pharmaceuticals**:** Chemistry, fate and transfer in the environment:

References:

1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
3. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
4. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
5. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
6. Environmental Chemistry, C. Baird, W. H. Freema
7. Latest review articles/research papers

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AC 10804 COMPUTATIONAL CHEMISTRY

Brief Idea about Quantum Mechanics:
Introduction, The Ultraviolet Catastrophe , The Photoelectric Effect ,The Quantization of the Electronic Angular Momentum, Wave-Particle Duality ,The Schrödinger Equation .,The Time-Independent, Schrödinger Equation, The Time-Dependent Schrödinger Equation, The Solution to the Schrödinger Equation

Basic Types of Modeling Techniques:
Force field (molecular mechanics), semiempirical, ab initio and density functional methods. Applicability, comparison of accuracy and cost. Thermodynamic ensembles: molecular dynamics and Monte Carlo techniques.

Basics of Electronic Structure Theory:
Atomic units. The qualitative role of kinetic and potential energy in shaping the orbitals. Treating spin as an extra dimension.

Roothaan-Hall Hartree-Fock method.
Energy expression with a Slater determinantal wavefunction. Basis set expansion of the orbitals. The Self-Consistent Field (SCF) method. Fock's theorem: invariance of the total wavefunction with respect to linear combination of occupied spin-orbitals. Hund's theorem and its implications.

Basis Sets.
Basis set types: atomic, plane wave and grid basis sets. Atomic basis sets: Slater-type and Gaussian functions. Some frequently used basis sets: minimum, double and triple zeta basis sets, polarization and diffuse basis functions. Major semiempirical techniques.

Molecular Properties And Wavefunction Analysis.
Orbital energies, Koopmans' theorem, electrostatic properties. Canonical and localized molecular orbitals and their use in qualitative understanding of molecular properties. Symmetry (briefly).

Density Functional Theory (DFT).
Discussion of DFT techniques. History, advantages and critique. Major exchange-correlation functionals.

The Calculation of Equilibrium Geometries, Force Constants, Vibrational Spectra, and Transition States. Gradient-based geometry optimization, the calculation of second derivatives, stability analysis. Reaction paths, the determination of transition states.

Electron Correlation.

Comparison of configuration-based and density functional (DFT) techniques. MP2, CI and Coupled Cluster methods. Static and dynamic electron correlation.
Mathematical derivations excluded

TEXTBOOKS:

1. F. Jensen Introduction to Computational Chemistry
2. D C Young Computational Chemistry
3. C J Carmer Computational Chemistry
4. K. I. Ramachandran · G. Deepa ·and K. Namboori, Computational Chemistry and Molecular Modeling

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AC 10805 SUPRAMOLECULAR CHEMISTRY

Introduction

Definition, host-guest chemistry, supramolecular interactions, interdisciplinary nature of supramolecular chemistry

Host-Guest Chemistry or Molecular Recognition

Classification of host molecules/receptors: cation and anion binding hosts; cation-binding hosts (crown ethers, podands, cryptands, spherands, calixarenes, siderophores), nomenclature, solution behaviour, selectivity of cation complexation, macrocyclic, macrobicyclic and template effects, preorganization and complementarity, soft ligands for soft metal ions, complexation of organic cations, alkalides and electrides; anion-binding hosts

Crystal Engineering

Concepts, crystal structure prediction, the cambridge crystallographic structural database, crystal engineering of diamondoid lattices, crystal engineering with H-bonds, H-bonds to carbon monoxide, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides, π-π stacking, other interactions, awkward shapes and mismatch, coordination polymers, biomimetic structures, mixed crystals: hourglass inclusions

Self-Assembly

Introduction, biochemical self-assembly, self-assembly in synthetic systems, self-assembling coordination compounds, self-assembly of closed complexes by hydrogen bonding, catenanes and rotaxanes, halicates, molecular knots, catalytic and self-replicating systems

Molecular Devices

Introduction, supramolecular photochemistry, information and signals: semiochemistry, molecular electronic devices: switches, wires and rectifiers, machine based on catenanes and rotaxanes, dendrimers

Biological Mimics

Introduction, characteristics of enzymes, cyclodextrins as enzyme mimics, corands as ATPase mimics, cation-binding hosts as Transacylase mimics, metallobiosites, haem analogues, vitamin B12 models

* The course will be offered as a pre-Ph.D course to the students who have not studied supra-molecular chemistry course at M.Sc.

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Reference Books

1. J. W. Steed and J. L. Atwood, "Supramolecular chemistry", John Wiley & Sons, Ltd, 2000.
2. F. Vogtle, "Supramolecular chemistry", John Wiley & Sons, Ltd, 1991.
3. J. W. Steed, D. R. Turner and K. J. Wallace, "Core concepts in supramolecular chemistry and nanochemistry", John Wiley & Sons, Ltd, 2007.
4. K. Ariga, T. Kunitake, "Supramolecular chemistry-fundamentals and applications", Springer-Verlag Berlin Heidelberg 2006.