DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY PATNA
PH.D. CHEMISTRY SYLLABUS

CH 701 SUPRAMOLECULAR CHEMISTRY **3 0 0 6**

Introduction to supramolecular chemistry (concepts and definitions), non-covalent forces and interactions in supramolecules, macrocycles and supramolecules (crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, porphyrins), self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, molecular devices and functional supramolecular structures – molecular wires, sensors, switches and logic gate devices, nano-scalar supramolecular reactors, metal-organic frameworks and their applications, nucleobases as supramolecular motifs, introduction to supramolecular liquid crystals and supramolecular gels, introduction to nanochemistry – nanoparticles and quantum dots.

Text:

1. J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, 2nd edition, John Wiley & Sons Ltd. (2009).

Reference:

1. J. W. Steed, D. R. Turner, K. Wallace, *Core Concepts in Supramolecular Chemistry and Nanochemistry*, 1st edition, Wiley, (2007).

2. H. Dodziuk, *Introduction to Supramolecular Chemistry*, 1st edition, Springer, (2001)

3. A. Katsuhiko, *Supramolecular Chemistry - Fundamentals and Applications*, 1st edition Springer, (2006).

CH 702 NEW REAGENTS FOR ORGANIC SYNTHESIS 3 0 0 6

Organotransition metal reagents: Principles, reagents developed from Titanium, Chromium, Iron, Rhodium, Nickel and Palladium. Introduction to non-metal reagents: Reagents containing Phosphorous, Sulphur, Silicon or Boron. Lanthanides in Organic Synthesis: General properties and use of Lanthanide metal compounds in different oxidation states in synthesis. Reagents from (i) Cerium (ii) Samarium (iii) Ytterbium. Oxidizing reagents: Use of reagent such as Pyridinium Chloro Chromate (PCC), Pyridinium Fluoro Chromate (PFC), Swern oxidation, DCC oxidation, Tetrapropyl ammonium peruthenate and other oxidizing agents. Reducing agents: Reductions involving $NaBH_4$, $LiAlH_4$, $NaBH_3CN$, DIBAL and Red –Al.

Text:

1. R. O. C Norman, J. M. Coxon, *Principles of Organic Synthesis*, 3rd edition, CRC Press, **(2009)**

2. T. Imamoto, *Lanthanides in Organic Synthesis*, Academic Press **(1994).**

3. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, 4th edition, Cambridge University Press, **(2006)**

4. J. Tsuji, *Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis*, John Wiley & Sons Ltd. **(2000)**

Reference:

1. P. G. Steel, "*Recent Developments in Lanthanide Mediated Organic Synthesis*," *J. Chem. Soc., Perkin Trans. 1*, **2001**, 2727-2751.

2. I. J. S. Fairlamb, "*Transition* Metals *in Organic Synthesis*," *Annu. Rep. Prog. Chem., Sect. B*, **2004**, *100*, 113-148.

3. G. A. Molander, "*Application of Lanthanide Reagents in Organic Synthesis,*" *Chem. Rev*., **1992**, *92*, 29-68

4. H. B. Kagan, J. L. Namy, "*Lanthanides in Organic synthesis*," *Tetrahedron*, **1986**, *42*, 6573-6614.

CH 703 SPECTROSCOPIC TECHNIQUES IN CHEMISTRY 3 0 0 6

Electronic Spectroscopy: General principles, Electronic absorption by molecules, absorption peaks and molar absorptivity, absorption and intensity shifts. Selection rules and their implications. Instrumentation: analytical applications: qualitative and quantitative analyses. Electronic spectra of inorganic and organic compounds. Infrared Spectroscopy: principles, factors influencing Vibrational frequencies, preparation of samples, the range of IR radiation, selection rules. Instrumentation: representation of spectra, dispersive and Fourier- transform IR–Spectroscopies. Application of IR Spectroscopy to inorganic and organic compounds. Raman Spectroscopy: principles, normal, resonance and laser Raman Spectroscopies. Structure determination by symmetry selection rules (normal coordinate analysis). Application of Raman Spectroscopy to structural chemistry; Nuclear magnetic resonance Spectroscopy: General principles, sensitivity of the method, CW and FT-NMR, Instrumentation. Application in chemical analysis (with special reference to 1H – NMR): Chemical shift, spin-spin splitting, area of peak, shift reagents, off-resonance decoupling, Nuclear Overhauser Effect, solid state and gas phase NMR spectra. Introduction to fluorescence, effects of solvents on fluorescence spectra, polarization of emission, measurements of fluorescence polarization. Timeresolved fluorescence Spectroscopy. Time dependent decays of fluorescence anisotropy. Mass spectrometry: Principles, advantages and limitations of Mass Spectrometry. Instrumentation, Methods of ionization, Metastable ions. Theory of Mass Spectrometry; Structure elucidation of inorganic and organic compounds; Mössbauer Spectroscopy: The Mössbauer Effect, the Mössbauer nuclei, chemical isomer shift, quadrupole splitting, magnetic hyperfine interaction. Elucidation of electronic structure of ^{57}Fe, ^{119}Sn compounds using Mössbauer data, Mössbauer of biological systems.

Text:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, *Introduction to Spectroscopy*, 3rd edition, Thomson Brooks/Cole, (2000)

2. C. N. Banwell, *Fundamentals of Molecular Spectroscopy*, 4th edition, Tata Magraw Hill, (1994)

3. R. M. Silverstein, G. C. Bassler, C. Morril, *Spectrometric Identification of Organic Compounds*, 5th edition, John Wiley & Sons, (1991)

4. J. R. Dyer, *Application of absorption Spectroscopy of organic compounds*, Prentice Hall of India Pvt. Ltd. (2004)

References:

1. R. S. Drago, *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, (1992)

2. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier, (1986)

3. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A & B, 5th edition, John Wiley & Sons Ltd., (1997)

4. M. Rose and R. A. W. Johnston, *Mass Spectrometry for Chemists and Biochemists*, 2nd edition, Cambridge University Press, (1996)

5. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd edition (2006)

CH 704 ART IN ORGANIC SYNTHESIS 3 0 0 6

Retrosynthetic analysis: Basic for retrosynthetic analysis, transforms and retrons, types of transforms, Biomimitic approach to retrosynthesis, Chemical degradation as a tool for retrosynthesis, Chiron approach. Transform-based strategies: transform-guided retrosynthetic search, Diels-Alder cycloaddition as a T-goal, retrosynthetic analysis by computer under T-goal guidance, enantioselective transforms as T-goals, mechanistic transform application, T-goal search using tactical combination of transforms. Structure-based and topological strategies: Structure-goal (S-goal) strategies, acyclic strategies disconnections, ring-bond disconnections-isolated rings, disconnection of fused-ring systems, disconnection of bridged-ring systems. Stereochemical strategies: stereochemical simplification-transform stereoselectivity, stereochemical complexity-clearable stereocenters, stereochemical strategies-polycyclic systems, Stereochemical strategies-acyclic systems. Functional group-based and other strategies: Functional group interconversion, functional group-keyed skeletal disconnections, disconnection using tactical sets of functional group-keyed transforms, strategies use of functional group equivalents, acyclic core group equivalents of cyclic functional groups, functional group-keyed removal of functional and stereocenters, functional group and appendages as keys for connective transforms. Use of several strategies: Multistrategic retrosynthetic analysis of longifolene, parontherine, perhydrohistrionicotoxin, Gibberellic acid, Picrotoxinin.

Texts:

1. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, 1st edition, Oxford University Press, (2001)

2. K. C. Nicolaou, E. J. Sorensen, *Classics in Total Synthesis*: *Targets, Strategies, Methods*, 1st edition, Wiley-VCH,(1996).

Reference:

1**.** E. J. Corey, X.-M. Cheng, *The Logic of Chemical Synthesis*, John Wiley & Sons Ltd, (1989)

2. M. B. Smith, *Organic Synthesis*, McGraw-Hill Inc., New York, (1994).

3. S. Warren, P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2nd edition, John Wiley & Sons Ltd, (2009).

CH 705 BIOANALYTICAL TECHNIQUES 3 0 0 6

Protein analysis & techniques: Protein purification methods: (ion-exchange, gel filtration and affinity chromatography), Protein estimation, Peptide mapping, Epitope analysis and mapping, Automated Peptide sequencing and synthesis. **Immunological Analysis:** Antibody production – Hybridoma technology, Western blot and Immunoprecipitation, Immunohistochemistry, Immuno-electrophoresis, Immuno-diffusion techniques, Immunoflourescence & Flow cytometry, Immunoassay: radioimmunoassay (RIA); enzyme-multiplied immunoassay technique (EMIT); fluorescence polarisation immunoassay (FPIA); closed enzyme donor immunoassay (CEDIA); enzyme-linked immunosorbent assay (ELISA), applications of immunoassays in diagnosis centers and screening of drugs. **Recombinant DNA Techniques:** automated DNA sequencing and synthesis, Techniques for the preparation of mRNA and cDNA, probes, Genome mapping, FISH (Fluorescent in-situ Hybridization), DNA fingerprinting (VNTR and micro satellite mapping), Gene cloning and expression: Cloning strategies, Production of recombinant proteins, Construction of DNA libraries, PCR methodology and applications, micro arrays. **Cell Technology Applications:** Cell & Tissue culture, DNA Transfections in eukaryotes: physical and chemical methods, Antisense technology and Large-scale cultivation of cells. **Electron microscopy in Bioscience:** Scanning Electron Microscopy (SEM), Transmission electron microscopy (TEM), Scanning Transmission electron microscopy (STEM) – basic technique and application in biomaterials characterization. **Electrophoresis applications:** Separation of Proteins, DNA, RNA (Agarose, Page, SDS-Page), gradient, 2-D Electrophoresis - CHEF, TAFE.

Texts:

1. Bioanalytical Techniques, M. L. Srivastava, Narosa Publishers.

2. Immunoassay and other Bioanalytical Techniques, Jeanette M. Van Emon, CRC Press, 2007.

Reference:

1. *Fundamentals of Bioanalytical techniques and Instrumentation*, Sabari Ghosal and A. K. Srivastava, PHI Learning.

2. *Gene Cloning- an introduction* (1995). T.A. Brown (3rd edition), Chapman & Hall, London

CH 706 INTRODUCTION TO COMPUTATONAL CHEMISTRY 3 0 0 6

Molecular Mechanics / Force Field Methods: Introduction to molecular mechanics; comparison of popular force fields; performance of molecular mechanics, review of postulates of quantum chemistry, The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states, variational method and principle, Hartree-Fock molecular orbital theory: Slater determinants, anti-symmetry principle, Hartree-Fock energy expressions for arbitrary spin-orbital configurations spin integration, restricted and unrestricted references, self-consistent-field (SCF) procedure, Basis sets: Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, correlation-consistent sets, core-valence sets, general contractions, basis set exchange, types of integrals, Gaussian product theorem, permutational symmetry of integrals, The Hartree-Fock algorithm, Semiempirical methods, Geometry optimization, Vibrational frequency analysis: symmetry analysis, harmonic vs. fundamental frequencies, zero-point vibrational energies (ZPVE's), Hessian index, distinguishing minima from transition states. Intrinsic reaction coordinates (IRC) analysis, analytic gradient theory, Electrostatics: atomic charges, dipole moment, polarizability, hyperpolarizability, Transition state theory, statistical mechanics, and thermodynamic properties, electron correlation, Configuration interaction, Many-body perturbation theory, Useful approximations: resolution of the identity (density fitting) and local correlation, Coupled-cluster theory, Density-functional theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, comparison of the performance of electronic structure theories.

Texts:

1. F. Jensen, *Introduction to Computational Chemistry*, 2nd Edition, Wiley, New York.

2. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st ed., revised, Dover, 1989.

Supplementary Books

1. D. A. McQuarrie, *Quantum Chemistry*, University Science Books, Mill Valley, CA, 1983.

2. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 3rd Edition.

CH 707: INTRODUCTION TO POLYMER SCIENCE & TECHNOLOGY **3 0 0 6**

Introduction to polymers, Molecular structure : Basic definitions, nomenclature and metrics; Polymerization chemistry and kinetics; Chemistry of additives; Characterization of molecular structure : Overview, intrinsic viscosity, GPC; Characterization of molecular structure; Glass transition; Super-molecular structure; Structure in blends and copolymers; Rheology; Processing and processing performance; Solid properties : Mechanical, tribological and others; Solid properties : Electrical, optical; Enhancing performance : Blends; Enhancing performance : Composites; Cases in materials selection / design and product design.

Suggested Readings

1) POLYMER SCIENCE AND TECHNOLOGY: Plastics, Rubbers, Blends and Composites- P. Ghosh, Publisher: *Tata Mc. Graw-Hill*

2) Seymour.Carraher's POLYMER CHEMISTRY- 7th Edition, *CRC Press*

3) Polymer Science and Technology, Joel R. Fried, 2nd Edition

4) Principles of Polymerization, George G. Odian, *John Wiley & Sons*

5) Physical Chemistry of Polymer Rheology - Furukawa, Junji, *Springer Series*

6) Polymer Synthesis and Characterization , Stanley Sandler, Wolf Karo, Eli Pearce, *Elsevier*

7) Textbook of Polymer Science, Billmeyer, 3rd Edition, *Wiley*

8) Polymer Science –V. R. Gowarikar.