DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

Departmental Elective Courses for the Ph D students

Course No. Subject L – T – P Credits
CH 601 Physical Methods in Chemistry 3 – 0 – 0 6
CH 602 Optical and Electronic Materials: A molecular Approach 3 – 0 – 0 6
CH 603 Supramolecules: Concept and Application 3 – 0 – 0 6
CH 605 Applied Crystallography 3 – 0 – 0 6
CH 610 Organometallics 3 – 0 – 0 6
CH 611 Bioinorganic Chemistry 3 – 0 – 0 6
CH 620 Art in Organic Synthesis 3 – 0 – 0 6
CH 621 New Reagents for Organic Synthesis 3 – 0 – 0 6
CH 630 A fundamental approach to Physical Chemistry 3 – 0 – 0 6
CH 631 Experimental Spectroscopy 3 – 0 – 0 6
CH 632 Chemical Applications of Group Theory 3 – 0 – 0 6
CH 638 Time Dependant Quantum Mechanics 3 – 0 – 0 6
CH 639 Principles and Applications of Molecular Fluorescence 3 – 0 – 0 6
CH 623 Chemistry of Biological Macromolecules 3-0-0-6
CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6

Detailed Syllabi
CH 601 PHYSICAL METHODS IN CHEMISTRY (3 0 0 6)
Pre-requisites: Nil

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, Selective Population inversion, Inter Nuclear Double Resonance (INDOR). Two dimensional and three dimensional NMR spectroscopies, Solid state and Gas phase NMR spectra, Polarization transfer techniques. 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. 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. 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. Mossbauer spectroscopy: The Mossbauer effect, the Mossbauer nuclei, chemical isomer shift, quadrupole splitting, magnetic hyperfine interaction. Elucidation of electronic structure of 57Fe, 119Sn etc. compounds using Mossbauer data; Mossbauer of biological systems. Chromatography: General principles, different types of chromatographic techniques, characteristics of working components and analytes.

Normal phase and reverse phase chromatography. Efficiency and resolution: Theoritical plate concept, van Deemter equation. Gas Chromatography: types of GC, basic components of GC, optimization of the method, GC-MS. Applications. High performance Liquid Chromatography: Different types of HPLC, basic components of HPLC, optimization of the method. Applications. Electrochromatography: Principles and applications. Thermal Analysis: General principles of thermal analysis. Thermogravimetric Analysis (TGA): Principles, instrumentation, study of thermogram, applications, limitations, DTG, Chemical Vapor Deposition (CVD), Metal Oxide Vapor Deposition (MOVD). Differential Thermal Analysis (DTA*):* Principles, instrumentation, study of thermogram, applications, limitations. Differential Scanning Calorimetry (DSC*):* Principles, instrumentation, study of thermogram, applications, limitations. Cyclic Voltammetry and Coulometry: Basic principles and applications to the study of electroactive species.

References:

1. R. M. Silverstein, G. Clayton Bassler and C. Morril, *Spectrometric Identification of Organic Compounds*, 5th Ed, John Wiley & Sons, 1991.
2. W. Kemp, *Organic spectroscopy*, 3rd Ed, ELBS, 1991.
3. R. S. Drago*, Physical Methods for Chemists*, 2nd Ed, Saunders College Publishing, 1992.
4. W. Kemp, *NMR in Chemistry: A Multinuclear Introduction*, Macmillan, 1986.
5. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Ed, 1986, Elsevier.
6. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A & B, John Wiley and Sons Inc., 5th Ed, 1997.
7. E. A. V. D. Ebsworth, D. W. H. Rankin and S. Cradock, *Structural Methods in Inorganic Chemistry*, 2nd Ed, Blackwell, 1991.
8. M. Rose and R. A. W. Johnston, *Mass Spectrometry for Chemists and Biochemists*, Cambridge University Press, 2nd Ed, 1996.
9. P. J. Haines, *Thermal Methods of Analysis—Principles, Applications and Problems*, Blackie Academic & Professional, 1st Ed, 1995.
10. G. D. Christian, *Analytical Chemistry*, John Wiley and Sons, 5th Ed, 1994.

CH 602 OPTICAL AND ELECTRONIC MATERIALS: A MOLECULAR APPROACH (3 0 0 6)

Pre-requisites: Nil

Overview of electronic devices, band theory, zone theory, conjugated systems, electronic excitation, chromophores, phosphorescence and fluorescence. Theories and application of one dimensional substances: electron-phonon coupling, Peirerls transition, solitons and polarons, superconductivity, conducting polymers, solution switching, molecular cellular automata, biocomputing, switching molecules, Langmuir Blodgett layers, holographic storage, light emitting diodes. Semiconductor devices, defect structures, p, n-type semiconductor, Structure property relations in high Tc superconductors. Chemical vapour deposition: Epitaxial growth, crystalline and amorphous films, metal organic vapour deposition, micro and nano crystalline materials. Ceramic materials. Electrochemistry of corrosion: thermodynamics of corrosion, Electrode kinetics, corrosion mechanism of electronic material systems, corrosion and protection. Fuel cells: Operational characteristic, power generation. Lithography: Principle, optical Lithography, deep-UV resists, multi layer systems, top surface imaging systems, Plasma etching, Dielectric and optical interconnects. Biological application of photochemical switches, Biosensors, Immunoassay, Neurotransmitters, fluorescence labels, Supramolecular devices, supramolecular electrochemistry, supramolecular ionics, molecular magnets, ion response monolayers, molecular channels, photohysteresis, dual mode photoswitching, self assembly of supramolecular liquid crystalline polymers, supramolecular material and composites.

Texts:

1. H. B. Pogge and Mercel Dekker (Ed), *Electronic Material Chemistry*, New York, 1996.
2. S. Roth, *One – dimensional metals: Physics and material science,* VCH, New York, 1995.
3. H. Morrission (Ed), *Biological application of photochemical Switches*, John Wiley, New York, 1993.

Reference:

1. J. M. Lehn, *Supramolecular Chemistry: Concept & perspective*, VCH, New York, 1995.
2. C. N. R. Rao and J. Gopalakrishnan, *New Direction in solid state Chemistry*, Cambridge University Press, 1997.
3. R. Arshahy (Ed.), *Desk reference of functional polymers: synthesis and application*; American Chemical Society, Washington, DC, 1996.
4. G. Burns, *High temperature superconductivity an introduction*, Academic press, New York, 1992.

CH 603 SUPRAMOLECULES: CONCEPT AND APPLICATION (3 0 0 6)

Pre-requisites: Nil

Definition, classifications of host guest compounds, thermodynamics and kinetic stability, role of weak interactions in supramolecules. Host design, preorganised hosts, complementarity, Cation, anion and neutral molecule binding hosts. Ionophores, receptors, recognitions, nano-dimensional hosts, supramolecular isomerism. Hydride sponge and related clathrates, inorganic solid state clathrates, layered solids, channel structures. Intracavity complexes of neutral molecules, crystal engineering, graph set analysis, co-ordination polymers, liquid crystals. Porous materials, surfactants. Supramolecular approach for chemistry-biology interface, neurotransmitters, optical sensing, switches, enzyme substrate binding, supramolecular catalysis, hydrophobic confinement in bio-mimicking molecules. Supramolecular green chemistry.

Texts:

1. J. W. Steedand J. L. Atwood, *Supramolecular chemistry*, Wiley, New York, 2000.
2. J. M. Lehn, *Supramolecular Chemistry*, VCH, New York, 1995.

3. H. J. Schneider and A. Yatsimirsky, *Principles and methods in Supramolecular chemistry*, Wiley, New York, 2000.

Reference:

1. J. L. Atwood, J. E. D. Davies, D. D. McNicol and F. Vogtle (Exe. Ed), *Comprehensive Supramolecular Chemistry*, Pergamon, New York, 1996.

CH 605 APPLIED CRYSTALLOGRAPHY (3 0 0 6)

Pre-requisites: Nil

Symmetry operations and space groups: Symmetry operations and symmetry in crystals, Crystallographic point groups, Space groups, Crystal lattice, Reciprocal lattice. Fundamentals of Diffraction Theory: Diffraction by a 3D-lattice, Bragg's law. X-rays: Origin, Production, Absorption, Filtering, Detectors, Selection of radiation. Crystals: Postulates of Crystallography (law of constancy of angles, law of rational indices), Crystal growth. Structure determination by X-ray crystallographic method: Choosing a crystal, Shaping a crystal, Crystal mounting, Optical alignment, Data collection, Data reduction, Phase problem, Refinement of crystal structures, Completing the structure. Neutron and Electron diffraction: Production and detection of neutrons, Neutron scattering factors, Special features of neutron diffraction, Production and detection of electrons, Electron scattering factors, Special features of electron diffraction.

Texts:

1. G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, The Macmillan Company, New York.
2. J. J. Rousseau, *Basic Crystallography*, John Wiley & Sons, New York, 1998.
3. Jenny P. Glusker, Mitchell Lewis and Miriam Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH, New York, 1994.
4. B. D. Cullity and S. R. Stock, *Elements of X - ray diffraction*, Prentice Hall, New Jersey, 2001.

References:

1. W. Massa, *Crystal Structure Determination*, Springer Verlag, Berlin, 2000.
2. W. Clegg, *Crystal Structure Analysis: Principles and Practice*, Oxford University Press, 2001.

CH 610 ORGANOMETALLICS (3 0 0 6)

Pre-requisites: Nil

Definition, classifications and bonding in organometallics. Isolobal analogies. Structural aspects of organometallics. Preparative methods. Spectroscopic techniques in organometallics chemistry. Electronic and magnetic properties of organometallic compounds. Stoichiometric and catalytic reactions: Fundamental process in reactions of organotransition metal complexes. Application of transition metal complexes to catalysis. Organometallics directed towards organic synthesis. Bio-organometallics, organometallics in environmental chemistry. Metal clusters and models for heterogeneous catalysis. Application of organometallics in industry.

Texts:
1. Yamamoto, *Organotransition metal in Chemistry, Fundamental concept and applications*; John Wiley, 1986.
2. R. H. Crabtree, *The organometallic Chemistry of the transition metals*, John Wiley, 1994.

CH 611 BIOINORGANIC CHEMISTRY (3 0 0 6)

Pre-requisites: Nil

Role of metal ions in Biology: Physiological effects of presence or absence of metal ions in biology. Role of ions in respiration, metabolism, photosynthesis and gene regulation in brief. Hard-soft Acid-Base Concept, Chelate effect, pKa values of coordinated ligand, redox potential, Nernst equation, Some kinetic aspects such as ligand exchange rate, substitution reactions and Electron Transfer Reactions. Brief description of peptide bond, primary, secondary and tertiary structure and hydrogen bonding. Various spectroscopic methods used in bioinorganic chemistry: Infrared, electronic spectra (specially d-d transitions), EPR (emphasis on first row transtion metal ions and their spectra), brief description of CD/MCD and multinuclear NMR. Brief descrieption and capability of newer methods like EXAFS, XANES, ENDOR. Classifications of metalloproteins and enzymes based on function with example: *Metalloproteins*; Dioxygen transport (Hemoglobin, Hemocyanin), Electron Transfer (Blue Cuprotiens, Cytochromes, Iron-sulphur protein), structural roles (zinc finger), uptake and storage proteins (ferritines). *Metalloenzymes:* Hydrolytic enzymes (zinc enzymes), redox enzymes (Binuclear redox enzymes, SODs photosystem II), oxygen-atom-transfer reactions (methane monooxygenase, catechol dioxygenase). Metalloproteins or enzymes either newly discovered or of current research interest not covered above should be included. Discussion about different approach employed in solving the problems in bioinorganic chemistry: Use of coordination complexes as model. Models for various enzymes will be discussed along with the above mentioned enzymes/proteins. Brief descriptions of other approaches like use of mutant enzymes. Topics of current interest: Thrust areas of research in bioinorganic chemistry such as role of nitric oxide and other topics will be discussed and student will participate writing a short report on one such topic and discuss in class.

Texts:
1. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, California. (Other journal articles and books will be referenced during the course.)

CH 620 ART IN ORGANIC SYNTHESIS (3 0 0 6)

Pre-requisites: Nil

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 Groupkeyed 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. E. J. Corey and Xue-Min Cheng, *The logic of chemical synthesis,* John Wiley, 1989.
2. M. B. Smith, *Organic synthesis,* McGraw-Hill Inc, New York, 1994.

CH 621 NEW REAGENTS FOR ORGANIC SYNTHESIS (3 0 0 6)

Pre-requisites: Nil

Lanthanides in Organic Synthesis: General properties of Lanthanides, use of Lanthanide metal compounds at different oxidation states in synthesis. Reagents from (i) Cerium (ii) Samarium (iii) Ytterbium etc. Organotransition metal reagents: Principles, reagents developed from Titanium, Chromium, Iron, Rhodium, Nickel, Palladium. Reagents containing Phosphorous, Sulphur, Silicon or Boron: Introduction, Phosphorous-containing reagents, Sulphur-containing reagents, Silicon-containing reagents,, Boron-containing reagents. Oxidising reagents: Use of reagent such as Pyridinium Chloro Chromate, Pyridinium Fluoro Chromate, Swern oxidation, DCC oxidation, Tetrapropyl ammonium peruthenate, other oxidizing agent. Reducing agents: Reductions involving (NaBH) 4, (LiAlH) 4, (NaBH)3CN, DIBAL, Red –Al.

Texts:

1. R. O. C Norman and J. H. Coxon, *Principle of Organic Synthesis*, 1st Ed, ELBS, 1993.
2. T. Imamoto, *Lanthenides in Organic synthesis*, Academic Press, 1994.
3. W. Carrutuer, *Some Modern methods of Organic Synthesis*, Cambridge, 1990.
4. L. W. Paqueette (Ed), *Reagents for Organic synthesis*, John Wiley, 1995.

CH 632 CHEMICAL APPLICATIONS OF GROUP THEORY (3 0 0 6)

Pre-requisites: Nil

Definitions and Theorems of Group Theory: Properties of Group and examples, Subgroups, Classes. Molecular Symmetry and the Symmetry Groups: Symmetry elements and Operations: symmetry planes and reflections, the inversion Center, Proper Axes and proper rotation, and Improper axes and improper rotations. Products of symmetry Operations. Equivalent symmetry elements and equivalent Atoms. General relations among symmetry elements and Operations. Symmetry Elements and Optical Isomerism. The symmetry point groups. Symmetries with multiple High- Order Axes. Classes of symmetry Operations. A systematic Procedure for symmetry Classification of molecules. Representations of Groups: Comments on Matrices and Vectors. Representation of groups. The "Great Orthogonality Theorem" and its consequences. Character Tables. Representation for Cyclic Groups. Group Theory and Quantum Mechanics: Wave function as bases for irreducible representations. The Direct Product. Detection of non–zero integrals. Symmetry Adapted Linear Combinations: Derivation of Projection Operators. Use of Projection Operators to construct SALCs. Molecular Orbital Theory and its Application in Organic Chemistry: General Remarks. Symmetry factoring of secular equations. Carbocyclic system. More general cases of LCAO-MO □□bonding. Naphthalene. Electronic excitations of Naphthalene: selection rules and configuration interaction. Three center Bonding. Symmetry based selection rules for cyclization reactions. Molecular Orbital Theory for Inorganic and Organometallic Compounds: Transformation Properties of Atomic Orbitals. Molecular orbitals for □□bonding in ABn molecules: The Tetrahedral AB4 cases. Molecular orbitals for □□bonding in ABn molecules.

Texts:

1. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Ed, John Wiley & Sons, 1990.

Reference:

1. F. L. Pilar, *Elementary Quantum Chemistry*, 2nd Ed, Dover Publications, INC, 1990.

CH 638 TIME-DEPENDENT QUANTUM MECHANICS (3 0 0 6)

Prerequisite: M.Sc. Chemistry or Physics.

Introduction; mathematical review; evolution operator: The Schrodinger, Heisenberg and interaction pictures; perturbation theory: Fermi's Golden Rule; numerical methods for wave packet representation and propagation: The Fourier grid, discrete variable representation, finite difference, split operator, Chebychev, Lanczos and the t,t' method; wave packet dynamics in harmonic oscillator; wavefunction auto-correlation: electronic wavefunction calculation, molecular spectra; two level system: Rabi oscillations; quantum tunneling: resonances; laser matter interaction: dipole approximation and the center of mass transformation, Gauge transformation, multiphoton interactions, above threshold ionization and dissociation, high harmonic generation; control of molecular dynamics; laser cooling and trapping.

Texts :

1. M. H. Mittleman, Introduction to the Theory of Laser-Atom Interactions, 2nd Edition, Plenum US, 1993
2. G. C. Schatz, and M. A. Ratner, Quantum Mechanics in Chemistry, Dover Publications, 2002
3. S. A. Rice, and M. Zhao, Optical Control of Molecular Dynamics 1st Edition, Wiley-Interscience, 2000

References :

1. N.B. Delone, and V.P. Krainov, Multiphoton Processes in Atoms, Springer Series on Atoms and Plasmas, Vol 13, Springer, 1994
2. A. Szabo, and N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, 1996
3. H. J. Metcalf, and P. van der Straten, Laser Cooling and Trapping 1st Edition, Springer, 2001

CH 623: Chemistry of Biological Macromolecules (3-0-0-6)

Prerequisite: none

Protein: amino acids, peptides, primary, secondary, tertiary, and quaternary structure of proteins, protein folding. Protein Synthesis: biosynthesis, chemical synthesis, solid phase peptide synthesis, Proteomics. Lipids: fatty acids, bilayer. Carbohydrates, Nucleic acids: base pairing, double helices, DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, Peptide nuclic acids (PNAs).

Texts:

1. A. Miller and J. Tanner, *Essentials of Chemical Biology*, Willey & Sons Ltd. 2008.
2. J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, W. H. Freeman and Company. 6 th Ed. 2007.

References:

1. S. L. Schreiber, T. Kapoor and G. Wess, *Chemical Biology: from small molecules to systems biology and drug design*, Wiley – VCH Verlag GmbH & Co. 2007.
2. C.M. Dobson, J.A. Gerrard and A.J. Pratt., *Foundations of Chemical biology*, OxfordUniversity Press. 2002

CH 639 Principles and Applications of Molecular Fluorescence 3 0 0 6

Absorption and emission of light, radiative and non-radiative transitions, fluorescence and phosphorescence emission, delayed fluorescence, laws of photochemistry, principles of steady-state and time resolved fluorometric techniques, time-domain and frequency-domain lifetime measurements, lifetimes and quantum yield, effects of solvents, temperature and molecular structure on fluorescence spectra, mechanisms of quenching, photoinduced electron and proton transfer, resonance energy transfer, fluorescence polarization, extrinsic causes of fluorescence depolarization, additivity law, free and hindered rotation, effect of rotational diffusion on fluorescence anisotropies: the Perrin equation, molecular probes and sensors, optical clinical chemistry and spectral observables and mechanisms of sensing.

Text Books:

1. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002.
2. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Ed. 2006.

References:

1. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 1: Techniques, Plenum Press, 1991.
2. J. R. Lakowicz, Topics in Fluorescence Spectroscopy, Vol. 4: , Probe Design and Chemical Sensing, Kluwer Academic Press, 1994.
3. B. Valuer and J. C. Brochon, New Trends in Fluorescence Spectroscopy: Applications to Chemical and Life Sciences, Springer, 2001.