INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE

POST B.Sc. INTEGRATED Ph.D. PROGRAMME IN CHEMICAL SCIENCES
(under the University of Calcutta)

Course Structure for M.Sc.

Notes:

1. "L+T" means 3 hours of lecture are followed by 1 hour of tutorial
2. "P" means practicals
3. For every course, course credits are equal to the number of contact hours per week

First Year

Semester I

Course Number	*Course Title*	*L+T - P*
CH411	Mathematics for Chemists	3–0
CH412	Quantum Mechanics	3–0
CH413	Inorganic Chemistry-I	3–0
CH414	Organic Chemistry-I: Structure and Dynamics	3–0
CH415	Biological Chemistry	3–0
CH416	Techniques in Chemistry-I	3–0
CH417	Laboratory	0–6

Total Contact Hours per week 24
Total Credits 24

Semester II

Course Number	*Course Title*	*L+T - P*
CH421	Symmetry in Chemistry	3–0
CH422	Equilibrium and Non-equilibrium Thermodynamics	3–0
CH423	Inorganic Chemistry-II	3–0
CH424	Organic Chemistry-II: Reagents and Reactions	3–0
CH425	Elementary Polymer and Solid State Chemistry	3–0
CH426	Numerical Methods and Computer Programming	2–1
CH427	Laboratory	0–6

Total Contact Hours per week 24
Total Credits 24

Second Year

Semester III

Course Number	*Course Title*	*L+T – P*
CH511	Equilibrium and Non-equilibrium Statistical Mechanics	3–0
CH512	Chemical Kinetics and Electrochemistry	3–0
CH513	Inorganic Chemistry–III	3–0
CH514	Organic Chemistry–III	3–0
CH515	Techniques in Chemistry-II	3–0
CH516	Research Project (With Seminar)	0–16

Total Contact Hours per week 31
Total Credits 31

Semester IV

Course Number	*Course Title*	*L+T - P*
CH521	Techniques in Chemistry-III	3–0
CH522	Elective-I	3–0
CH523	Elective-II	3–0
CH524	Elective-III	3–0
CH525	Elective-IV	3–0
CH526	Research Project Continued (With seminar)	0–16

Total Contact Hours per week 31
Total Credits 31

DETAILED COURSE CONTENTS

FIRST YEAR: SEMESTER I

CH 411: Mathematics for Chemists

- ***Ch-1:(3L)*** Function: functions, limits, continuity, Integral and differential calculus of one and two variables, Mean Value Theorems, Improper Integrals, Convergence of Integrals.
- ***Ch-2:(4L)*** Infinite series and sequences: convergence and divergence of infinite series, Tests of convergence, alternate series, Taylor series and application, Asymptotic expansion and application, Fourier sine and cosine series and applications,
- ***Ch-3:(2L)*** Functions defined as integrals: Gamma, Beta and error functions, exponetial integrals, elliptic integrals, Dirac delta functions
- ***Ch-4:(4L)*** Linear algebra and Vector spaces: Matrices, Rank of a Matrix, Complex Inner Product Spaces, Orthogonal and Unitary Transformations, Eigenvalues and Eigenvectors and application, Change of Basis, Diagonalization of Matrices.
- ***Ch-5:(5L)*** Complex variables: Limits, continuity, Differentiations, Cauchy-Reimann equations, Complex integrations, Residues and Cauchy residue theorem.

  Laplace inversion, Evaluation of real, definite integrals,
- ***Ch-6:(4L)*** Differential equation: Methods of solution, Laplace transformation method, Power series method, Fourier expansion methods.
- ***Ch-7:(3L)*** Orthogonal polynomials: Orthogonal polynomials, Legendre and Hermite polynomials, Sturm-Liouville Theory, Eigenfunction Expansions.
- ***Ch-8:(4L)*** Partial differential equation: Examples, chain rule, Laplace equation in Cartesian and polar form, one and two dimensional wave equations, Heat equations,
- ***Ch-9:(4L)*** Vectors: Definitions, dot product, cross product, vector fields, Differentiation, line integrals, surface integrals, Divergence Theorem, Stokes Theorem, Tensors(qualitative concepts), summation convention and co-ordinate transformation.
- ***Ch-10:(4L)*** Nonlinear Differential equations: Phase plane, fixed points, linear stability analysis, vanderPol oscillator and limit cycle, Population dynamics.
- ***Ch-11:(3L)*** Probability and Statistics: Laws of probability: compound events, mutually exclusive events and statistically independent events. Mean and standard deviation of Binomial distribution, Poisson distribution and Gaussian distribution.

- ***Ch-12:(2L)*** Curvilinear Coordinates: Plane Polar Coordinates, Vectors in Plane Polar Coordinates, Cylindrical Coordinates, Spherical Coordinates, Curvilinear Coordinates.

Suggested Books:

1. *Applied Mathematics for Scientist and Engineers, Pipes and Harvill, MCGraw Hill, 1971*
2. *Mathematical Methods for Scientists and Engineers, D. A. McQuarrie University of California, Davis*
3. *Mathematical methods for Physicist, Arfken and Weber, Academic, 1995*
4. *Advanced Engineering Mathematics, Kreyszig (Wiley).*
5. *Methods of Mathematical Physics, Courant and Hilbert Wiley, 1989.*

CH 412: Quantum Mechanics

- Sequence of events/phenomena which establish that (i) both radiation and matter have wave-particle duality and (ii) physical variables can be discrete/quantized. Elementary classical mechanics, using linear harmonic oscillator(LHO) as an example. Trajectories in configuration space and phase space. Lagrange's and Hamilton's equations of motion. Poisson's bracket. Classical wave equation. Plane-wave solutions. De Broglie matter waves. Operators. Linear Operators. The eigenvalue problem; occurrence of quantization, bounded and unbounded systems, discrete and continuous eigenvalue spectra. Commutation relations, commuting and non-commuting operators, eigenfunctions.
- Probability distribution(weighting function) and expectation value. Operations of observation and their properties; parallelism with commuting/non-commuting eigenoperators. "Small" and "large" systems; origin of uncertainty and connection to commutation relations.
- Postulates of quantum mechanics and their interpretations. Schroedinger equation and various interpretations of equation, energy spectrum, wave functions(Hilbert space), operators and Dirac notation(vectorial analogy). Hermitian operators. Acceptability conditions restricting energy values. Proof of Uncertainty Principle. Parity of eigenfunctions. Ehrenfest theorem. Heisenberg equation of motion.
- Applications to one-, two- and three-dimensional systems, degeneracy, Jahn-Teller effect. LHO(in terms of ladder/creation-annihilation operators), rigid rotor(including electron in a ring), hydrogen atom(ladder operators). One-dimensional periodic potential; Bloch theorem, band structure.
- Angular momentum in quantum mechanics in terms of ladder operators. Electron spin; Pauli spin matrices. Spin and magnetic field. Exchange; Slater determinant. Spin-orbit coupling. Spectral term symbols.
- Approximate methods: Time-independent and time-dependent perturbation theories ; their applications. The variation principle for ground and excited states. Linear variation method and its applications: MO theory, VB theory, Hueckel MO theory;
- Hartree, Hartree-Fock and Hartree-Fock-Roothaan methods. Electron correlation. Configuration interaction; natural orbitals. Born-Oppenheimer approximation. Semiempirical methods.
- Electron density. Density matrices; Elementary introductions to density functional theory (including Thomas-Fermi-Dirac-Weizsaecker theory).

Suggested Books:

1. *I. N. Levine, Quantum Chemistry, Prentice-Hall-India.*
2. *D.W. McQuarrie, Quantum Chemistry, Oxford University Press.*
3. *P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press.*
4. *A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover.*
5. *F. L. Pilar, Elementary Quantum Chemistry, McGraw-Hill (1968).*
6. *R. McWeeny and B.T. Sutcliffe, Methods of Molecular Quantum Mechanics, Academic Press. 10*
7. *P. W. Atkins, Quanta: A Handbook of Concepts, Oxford University Press.*
8. *G. C. Schatz and M.A. Ratner, Quantum Mechanics in Chemistry, Prentice Hall.*
9. *F. Schwabl, Quantum Mechanics, Narosa Publishing House*
10. *L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Butterworth-Heinemann.*

CH413: Inorganic Chemistry- I

- **Structure and Reactivity of Inorganic Molecules:** Bonding models in inorganic chemistry–ionic and covalent bonds; chemical forces; acid-base chemistry; chemistry of aqueous and non-aqueous solvents-electrode potential and electromotive forces.

- **Basic Principles of Coordination Chemistry:** Coordination number and ligand polytopes, isomerism in coordination complexes, transition metal chemistry, principles of coordination chemistry related to bioinorganic chemistry and material chemistry.

Suggested books:

1. *James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity (4th Edition), Publisher: Benjamin Cummings.*
2. *Douglas, McDaniel and Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed, Wiley, New York, 1994.*
3. *Gary Wulfsberg, Inorganic Chemistry, University Science Books, USA.*
4. *A. von Zelewsky, Stereochemistry of Coordination Compounds, J. Wiley & Sons, 1996.*

CH414: Organic Chemistry-I: Structure and Dynamics

- Conformational analysis of acyclic and cyclic structures; concept of symmetry, chirality, topicity; structure and reactivity
- Frontier orbitals in organic reactions; orbital symmetry and pericyclic reactions; control of stereochemistry and secondary orbital interactions; Lewis acid catalysis and selectivity
- Reaction mechanism; physical methods of determination of reaction mechanism; rearrangement reactions in the context of ring-transformation and stereochemistry; transition state models for nucleophilic addition to carbonyl groups
- Organic photochemistry; Principles and reactions - photolytic cleavage, photoreduction, photooxidation, photoaddition, photorearrangement
- Reactive intermediates; carbenes and nitrenes; SET pathways

- Chemistry of free radicals; generation and bond-forming reactions; stereoselectivity

Suggested books:

1. *Advanced Organic Chemistry, 5th ed. Part A: Structure and Mechanisms – F.A. Carey and R. J. Sundberg, Springer, 2007.*
2. *Stereochemistry of Organic Compounds – E. L. Eliel and S. H. Wilen, John Wiley, 1994.*
3. *Modern Molecular Photochemistry of Organic Molecules – N. J. Turro, V. Ramamurthy and J. C. Scaiano, University Science Books, 2010.*
4. *Free Radicals in Organic Chemistry - Jacques Fossey, Daniel Lefort and Janine Sorba, Wiley, 1995.*
5. *Advanced Free Radical Reactions for Organic Synthesis – H. Togo, Elsevier, 2004.*
6. *Reactive Intermediates in Organic Chemistry – N. S. Isaacs, John Wiley, 1975.*

CH415: Biological Chemistry

- ***Chemical principles of life (8L)***
    1. Chemical principles that govern the processes driving living systems
    2. Chemistry of carbohydrates, lipids and hormones
    3. Chemistry of amino acids, peptides and proteins
    4. Chemistry of Heterocycles: nucleosides, nucleotides and nucleic acids
    5. Structure of macromolecules: Proteins, DNA, RNA
- ***Enzyme kinetics (6L)***
    1. Enzyme action: transition state theory,
    2. Examination of the kinetics of single and multi-substrate enzyme reactions,
    3. Kinetics and mechanisms of reversible and irreversible inhibition with special reference to potent inhibitor design,
    4. Allosterism.
- ***Fundamentals of cell biology (9L)***
    1. Structure and function of cell organelles.
    2. Modern aspects of molecular basis of cell function: cell migration, secretion, division and intercellular communication.
    3. Chromosome structure and function, nucleosomes,ribosomes and biological membranes
- ***Introduction to Molecular Biology (9)***
    1. Foundations of Molecular Biology. Replication: chemistry and topology, DNA recombination and DNA damage.
    2. Transcription: mechanisms in prokaryotes and eukaryotes, RNA splicing, RNA editing and RNA interference.
    3. Translation: protein biosynthesis, genetic code, gene expression and its regulation
- ***Techniques in modern biology (8)***
    1. Introduction to bio-softwares.
    2. Introduction to Gel electrophoresis.
    3. Introduction to microscopy in Cell biology

Suggested books:

Biochemistry:

1. Lehninger, Nelson, Cox
2. Voet, Voet
3. Stryer

Biophysical Chemistry:

1. Cantor, Schimmel
2. Tinoco, Wang
3. van Holde

Molecular Biology of the Cell:

1. Baltimore, Lodish, Darnell
2. Alberts

Genetics:

1. Suzuki
2. Russell
3. Gardener
4. T.A.Brown

Enzymes:

1. Alan Fersht

CH416:Techniques in Chemistry- I

- Basic electronics and instrumentation

- Structure Elucidation of Organic Compounds:

  UV spectroscopy: chromophore, Beer's law, Woodward's rules, quantitative analysis
  Infrared spectroscopy: Basics, Determination of functional groups
  ^{1}H NMR and ^{13}C NMR spectroscopy: Basic principles, chemical shifts, coupling constants, spin coupling, geminal/vicinal coupling constants, integration, virtual coupling, long range coupling, diastereotopic protons, Karplus correlation, Nuclear Overhauser effects, 2-D-correlation spectroscopy.

- Mass spectrometry: Ionization techniques (EI, CI, DI, SI), FAB, MALDI, mass analyzers, fingerprint applications, interpretation of mass spectra, isotope distribution.

- Chromatographic techniques: principles of chromatography, gas chromatography, high performance liquid chromatography.

- Electroanalytical methods

- Termoanalytical techniques: Thermogravimetric analysis, Introduction, Instrumentation, Factors affecting thermogravimetric results, applications of Thermogravimetry. Differential Thermal analysis and differential scanning calorimetry.

Suggested books:

1. *H. H. Willard, L. L. Merritt, Jr., J. A. Dean, F. A. Settle, Jr., Instrumental Methods of Analysis.*
2. *R. M. Silverstein, F. X. Webster, Spectrometric Identification of Organic Compounds.*

CH 417: Laboratory

- Experiments will be chosen from Chemistry, Physics and Biology and should be interdisciplinary in nature
- Experiments may vary from year to year depending upon the interests of the students and expertise of the instructor.

COURSE CONTENTS

FIRST YEAR: SEMESTER II

CH 421: Symmetry in Chemistry

Symmetry as a mathematical concept; symmetry and physical properties of atoms, molecules and solid, symmetry, quantum mechanics and conservation laws.

Symmetry in chemical sciences explored through group theory.

Elements of group theory in chemistry: Symmetry operations and their associated algebra. Dipole moment and optical activity. Group, subgroup, symmetric(permutation) group, simple group, semi-simple group, colour(magnetic/Shubnikov)group, point group, space group. Isomorphism and homomorphism. Properties of groups. Schoenflies notation for point groups. Hermann-Maugin notation for space groups. Generating elements of a group. Elementary theory of representations of groups; transformation operators, function spaces, invariant subspaces. Equivalent, reducible and irreducible representations. Character tables(grand orthogonality thorem, other theorems/relations involving irreducible representations and characters). The reduction of a representation; projection operators. Notations for character tables for point groups. Definition of an algebra. Direct product group; direct product representation. Representations and quantum mechanics. The vanishing of integrals. Applications of group theory to bonding, structure and reactivity as well as other properties: Symmetry-adapted MOs of small and medium-size molecules(e.g., benzene, MX6, etc), Mulliken-Walsh correlation diagrams. Molecular vibrations(normal modes and normal coordinate 18 analysis).“Proof”of Jahn-Teller theorem; first- and second-order Jahn-Teller effects. Selection rules for single- and two-photon spectroscopy of various types, intensity “borrowing”, magnetic dipole selection rules. Woodward-Hoffmann and FMO approaches to reactivity. Symmetry selection for transition states and reaction paths.

***Suggested books**:*

1. *D. M. Bishop, Group Theory in Chemistry, Dover.*
2. *F. A. Cotton, Chemical Applications of GroupTheory, John Wiley.*
3. *J. M. Hollas, Symmetry in Molecules, Chapman*
4. *I. Hargittai and M. Hargittai, Symmetry Through the Eyes of a Chemist, Plenum Press.*
5. *M. Tinkham, Group Theory and Quantum Mechanics, McGraw-Hill.*
6. *C. D. H. Chisholm, Group Theoretical Techniques in Quantum Chemistry, Academic Press.*
7. M. Hamermesh, Group Theory and Its Applications to Physical Problems, Dover.

CH 422: Equilibrium and Non- equilibrium Thermodynamics

A. Equilibrium Thermodynamics

- Concept of thermodynamic equilibrium: Thermal, Mechanical and Chemical Equilibrium (2L)
- Formal relationships: Euler equation; Gibbs-Duhem relation (1L)
- Maximum work Theorem: Maximum Entropy an Minimum Energy principle (2L)
- Legendre transformation and thermodynamic potentials; Minimum principles of potential (3L)
- The Maxwell relations and simple applications (1L)
- Stability condition for thermodynamic potential (3L)
- First order phase transition; Clausius-Clapayron equation; Gibbs Phase rule (3L)
- Thermodynamics in the neighborhood of the critical point with emphasis on scaling and universality (3L)
- Thermodynamics of small systems: Emphasis on interfacial energy (NVT ensemble) (1L)

B. Statistical Thermodynamics

- Ensemble and Ensemble averages, Partition function and thermodynamic potential (2L)
- Electronic, translational, vibrational and rotational partition function for hetero and homo nuclear diatom (2L)
- Calculation of equilibrium constant (1L)

Suggested books:

1. H. B. Callen, Thermodynamics & Introduction to Thermostatistics
2. T. C. Hill, Thermodynamics of small systems
3. K. G. Denbigh, Principles of Equilibrium Thermodynamics

C. Non-Equillibrium Thermodynamics

- Conservation laws; entropy production and 2^{nd} law of thermodynamics (3L)
- Flux and thermodynamic force; Phenomenological equations; Onsager's reciprocal relations (4L)

- Stationary states; states with minimum entropy production; Glansdorf-Prigogine inequality (3L)
- Boltzmann equation, hydrodynamics, H-theorem (2L)
- Applications: Unimolecular reactions; Ion transport in Biological systems; spinodal decomposition (3L)

1. Bifurcation and symmetry breaking: Turing pattern in autocatalytic systems; Brusselator; Predator-prey model; morphogenesis (4L)

Suggested books:

1. *S. R. de Groot and P. Mazur, Non-equilibrium Thermodynamics*
2. *I. Prigogine, Introduction to thermodynamics of irreversible processes, Interscience Publishers; 2d, rev. ed edition (1961)*
3. *I. Prigogine, From Being to Becoming: Time and complexity in the physical sciences, Freeman, San Francisco, 1980.*
4. *D. Mcquarrie, Statistical Mechanics, Harper, NY, 1976.*
5. *H.J. Kreuzer, Nonequilibrium Thermodynamics and its Statistical Foundations, Clarendon, 1981, Oxford*
6. *D Avnir, Fractal Approach to Heterogeneous Chemistry: Surfaces Colloids and Polymers, John Wiley & Sons, NY, 1989.*
7. *J Keizer, Statistical Thermodynamics of Nonequilibrium Processes, Springer-Verlag, Berlin, 1987. 12*

CH 423: Inorganic Chemistry-II

- **Organometallic Chemistry**: 18-electron rule, electron counting in complexes, metal carbonyl complexes, phosphines, carbonyl hydride complexes, carbene, carbyne and carbide complexes, Fischer carbene and Schrock catalyst, Grubb's catalyst: olefin metathesis, alkene and alkyne complexes, arene complexes, Metallocenes, Nitrosyl and dinitrogen complexes, Reactions of organometallic complexes, Catalysis by organometallic complexes: Wilkinson's catalyst in alkene hydrogenation, synthetic gas, Hydroformylation, Wacker process, synthetic gasoline, Ziegler-Natta catalysis.

- **Bonding and Spectra of Coordination Compounds**: MO theory: Oh complexes, Td and SP complexes, Pi bonding, MO of organometallic complexes, Electronic spectra, Orgel diagram, Tanabe-Sugano diagrams, Jahn-Teller distortion, CT spectra.

- **Molecular magnetism:** Magnetization and magnetic susceptibility. Magnetic properties of transition metal complexes, magnetism in exchange coupled system, magnetic properties of lanthanides and actinide complexes. Molecules containing a unique magnetic center with a first-order angular momentum. Isotropic interaction in dinuclear compounds. Orbital models of the exchange interaction: case of two local doublet states. Magnetic chain compounds. Magnetic long-range ordering molecular compounds: design of molecular-based magnets. Spin-dependent delocalization in mixed-valence compounds.

- **Inorganic Chains, Rings, Cages, and Clusters**
  Chains: Catenation, Heterocatenation, Silicates, Intercalation chemistry, Isopoly, heteropoly anions. Rings: Borazines, Phosphazenes. Cages: Boron cage compounds,

Carboranes, Metallacarboranes. Metal clusters: Dinuclear, Trinuclear, Tetranuclear, Hexanuclear compounds, Zintl phases.

Suggested books:

1. *Douglas, McDaniel and Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed, Wiley, New York, 1994.*
2. *James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity (4th Edition), Publisher: Benjamin Cummings.*
3. *Lukehart, C.M., Fundamental Transition Metal Organometallic Chemistry.*
4. *R. H. Crabtree, The Organometallic Chemistry of the Transition Elements, J. Wiley & Sons, 1988.*
5. *Inorganic Electronic Structure and Spectroscopy Vol I: Methodology, Ed. By E. I. Solomon, A. B. P. Lever, John-Wiley and Sons, Inc.*
6. *Inorganic Electronic Structure and Spectroscopy Vol II: Applications and Case studies, Ed. By E. I. Solomon, A. B. P. Lever, John-Wiley and Sons, Inc.*
7. *Physical methods in Chemistry, R. S. Drago, W. B. Saunders Company.*
8. *A. Earnshaw, Introduction to Magnetochemistry, Academic Press. London, 1968*
9. *A. F. Orchard, Magnetochemistry, OUP, (OCP No. 75), 1999.*
10. *O. Kahn, Molecular Magnetism.*

CH 424: Organic Chemistry II: Reagents and Reactions

- Reducing agents, Birch reductions, Oxidizing agents
- Protecting group chemistry
- Wittig olefination and Horner-Wadsworth-Emmons Olefination
- The Olefin Metathesis Reaction
- Pd-mediated carbon-carbon bond formation
- Directed ortho-metallation and Grignard reaction
- Selective name reactions (Bamford-Stevens reaction, Eschenmoser Fragmentation, Mitsunobu reaction, Macrocyclization, Stuadinger reaction or ligation, Baldwin's rule for ring closure, Michael reaction, Robinson's annelation, Curtius rearrangement, Iodolactonization or halolactonization, Fischer indole synthesis, Larock's heteroannulation, Dihydroxylation of olefins), Umpolung effect.
- Epoxidation and aziridination reactions
- Use of DCC, HOBt, HOAt, HBTU for peptide synthesis
- Combinatorial chemistry and diversity oriented synthesis (DOS).
- Useful reactions in bioconjugation chemistry

Suggested books:

1. Modern Methods in Organic Synthesis by W. Carruthers.
2. Modern Synthetic Reactions by H. O. House.
3. Advanced Organic Chemistry by J. March.
4. Advanced Organic Chemistry (Part B) by F. A. Carey and R. J. Sundberg.
5. Organic Synthesis by M. B. Smith.
6. Comprehensive Organic Transformations by R. J. Larock.
7. Protective Groups in Organic Synthesis by T. W. Greene.

Online sources: *1. Sci Finder.*
2. Web of Science.
3. Electronic Journals.
4. EROS (Encyclopedia of Organic Reagents – online)

CH 425: Elementary Polymer and Solid State Chemistry

A. Basic Polymer Chemistry

- **Introduction to polymers (2L):** Natural polymers; synthetic polymers; structures of commonly used polymers; various terms (average molecular weight, number average, weight average, polydispersity index etc.) used in polymers literature.
- **Classification of polymers based on various parameters (1L):** Stereochemistry, structure, crystallization nature etc.
- **Synthesis of polymers (10L):** Step growth polymerization- various polymerization reactions, control of molecular weight (mono-functional impurity, stoichiometric imbalance); Chain polymerization- radical polymerization, mechanism, kinetics, reactivity ratios, various ring-opening polymerization, ionic polymerization, coordination polymerization; Introduction to controlled ("living") polymerization- ATRP, RAFT, NMP, GTP; Emulsion polymerization, precipitation polymerization.
- **Branched polymers (2L):** Hyperbranched polymers, dendrimers.
- **Polymer Characterization (5L):** Thermal analysis (glass transition temperature, crystalline melting temperature); Mechanical properties (Elastomers, fibres, thermoplastics etc.); Determination of molecular weight (end group analysis, GPC, viscosity, VPO).

Suggested books:

1. Principles of Polymerization: George Odian
2. Introduction to Polymer Science and Chemistry: Manas Chandra
3. Principles of Polymer Chemistry: P. J. Flory
4. Textbook of Polymer Science: F. W. Billmeyer.

B. Solid state Chemistry

- Structure of Solids: Periodicity, Fundamental lattice types (two & three dimensional), Index systems of crystal planes, Crystal structures and close packed arrangements, Diffraction, Bragg's Law, Reciprocal Lattice Vectors, Diffraction Condition, Laue Equation & Brillouin Zones. (3L)

- Crystal Vibrations & Phonons: Vibrations with monatomic basis, Group velocity & its relation to sound velocity at long wavelength limit, Elastic Strains, Compliance & Stiffness Constants, Elastic Waves. Derivation of Force constants from experiments, Normal modes, Density of States in one & three dimensions, Debye T^3 Law. (4L)

- Band Theory and Electronic Structure of Solids, Tight Binding Model (2L)

- Deviations from Ideal Crystals (descriptive): Crystal Defects, grain boundaries, dislocations, stacking faults and reactivity of solid due to the non-ideal structure; Glassy and amorphous materials, Alloys (3L)

- Tailor-making of materials with desired properties: (10L)

  a. Materials like liquid crystals /surfactant, microemulsions and micelles/colloids/polymer/membrane:
  Liquid crystals: Chemical synthesis; ordering of phases: isotropic, nematic and smectic (descriptive); Maier-Saupe model for isotropic-nematic phase transition; anchoring.

  Colloid: Chemical synthesis; colloidal phases (descriptive); screened Coulomb interaction in charged colloid, phase transition in colloids and colloids under shear (descriptive).

  Biological membranes (simple description of Mosaic model).

  b. Superconducting Materials: Basic phenomenologies of type I and type II superconductors, BCS theory, phenomenology of high Tc superconductors
  c. Quasi-one dimensional systems (phenomenology only)
  d. Charge ordering systems (phenomenology)
  e. Nanomaterials: Nanotubes, Fullerenes (descriptive)

Suggested books:

1. *Solid State Chemistry & Its Applications by A. R. West (John Wiley & Sons)*
2. *New Directions in Solid State Chemistry by C N R Rao & J. Gopalakrishnan (John Wiley & Sons)*
3. *Crystal Chemistry and Physics of Metals and Alloys by W. B. Pearson (Wiley 1972)*
4. *Introduction to Crystal Geometry by M. J. Buerger (McGraw-Hill, 1971)*
5. *Phonons: Theory and Experiments by P. Bruesch (Springer 1987)*
6. *Structural Phase Transitions by A. D. Bruce and R. A. Cowley, (Taylor & Francis, 1981)*
7. *Thermal expansion of crystals by R. S. Krishnan (Plenum, 1980)*
8. *N. W. Ashcroft and N. D. Mermin, 'Solid State Physics', Saunders College Publishing*
9. *de Gennes*
10. *T. C. Chaikin and T. C. Lubensky, 'Principles of Condensed Matter Physics', Cambridge University Press*
11. *Safran*

CH 426: Numerical Methods and Computer Programming

Programming Language:

- Basic knowledge of C or Fortran 90 – Data statements, Logical and Arithmetic expressions, Operators, I-O statements, Implementation of Loops, Control Statements, Functions and Subroutines, Array manipulation, Processing Strings

and Characters, Format Specifications, File processing, Derived types, Pointers and Structure Data Type.

- Familiarization with Linux based operating system, development of simple C or Fortran programs, compilation and execution.

Numerical Methods:

- Root finding of equations having numerical coefficients using Successive Bi-section and Newton Raphson method
- Basic ideas of Interpolation – Newton's forward and backward interpolation, Lagrange method for unequal intervals
- Numerical integration of a definite integral using Trapezoidal and Simpson's one-third rule
- Statistical Description of Data
- Fast Fourier Transform, Fourier and Spectral Applications
- Numerical solution for a set of coupled ordinary differential equation –
- Initial Value Problem: Runge Kutta Method, (ii) Boundary Value Problem: Relaxation Technique, ShootingMethod
- Partial Differential Equations (PDE): (i) Elliptic PDE – Static Boundary Value Problems, (ii) Parabolic PDE – Time Evolution or Dynamic Initial Value Problems, (iii) Hyperbolic PDE – Wave Propagation Problems

Practicals:

Modeling in:

a. Chemistry:
b. Physics: e.g. Montecarlo/Cellular automata/Randomwalk/Boundary value problem etc.
c. Biology: Position determination in biological systems, Checkpoint regulation in Mitosis,

Suggested books:

1. *Applied Numerical Analysis: Gerald and Wheatley, Pub:Pearson*
2. *An introduction to computational physics: Tau Pang, Cambridge Univ. Press*
3. *Introduction to Numerical Methods and FORTRAN Programming: Thomas Richard McCalla, John Wiley and Sons Ltd*

CH 427: Laboratory

- Experiments will be chosen from Chemistry, Physics and Biology and should be interdisciplinary in nature
- Experiments may vary from year to year depending upon the interests of the students and expertise of the instructor.

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COURSE CONTENTS

SECOND YEAR: SEMESTER III

CH 511: Equilibrium and Non-equilibrium Statistical Mechanics

- **Equilibrium Statistical Mechanics**

1. Random Events, Probability and probability distributions, Binomial, Poissonoian and Gaussian distributions, Fluctuations and dissipation, Central limit theorem, Maxwell's momentum distribution law in field free space, Principle of detailed balance and equilibrium Maxwell – Boltzmann distribution, Classical Gibbs distribution and thermodynamic properties, Equipartition theorem, Quantum canonical and grand canonical Gibbs distribution.
2. Ideal Bose Gas: Photon Statistics, Specific heat of insulators, and BE condensation.(3L)
3. Ideal Fermi Gas: Specific heat ofd free electron gas (2L)
4. Exact Solution of 1-D Ising model via Transfer Matrix; Mean Field Solution of 3-D Ising Model. (2L)
4. Concept of order parameter through magentic phase transition; Landau theory for continuous phase transition and its connection to Mean Field solution of Ising model; First Order phase transition with illustration via Isotropic-Nematic phase transition. (3L)
5. Elementary theory of Liquid Structures: Definitions of single particle density, two particle density, pair correlation function and structure factor; Relation between pair correlation function and structure factor; Experimental significance of structure factor; Equation of state of a liquid; Mean Field treatment of electrolyte solution. (5L)
6. Computer Simulation: statement of basic algorithm of MC and MD. (The instructor may enecourage students to perform simulation on simple systems, for e.g., Ising system, Lennard-Jones fluid etc). (2L)

- **Nonequilibrium Statistical Mechanics**

1. Stochastic Processes and Transition Probability; Random Walk: Master Equation of diffusion over a lattice; Time dependent correlation function, response function, Linear response and susceptibility with illustration via harmonic oscillators; Fluctuation-Dissipation theorem. (7 lectures)
2. Slow and fast degrees of freedom: Illustration via damped harmonic oscillator; Elementary idea of elimination of fast degree of freedom and noise; Langevin Equation of motion of Brownian particle and calculation of different correlation functions; Over damped dynamics with illustration from the Rouse Model of polymer chain. (4 lectures)
3. Phenomenological formulation of equation of motion for conserved and nonconserved modes (model A and model B). Transport coefficient. Linearised hydrodynamics of simple fluids: diffusive and propagating modes. (4 lectures)

Suggested books:

1. *Plischke and Bergerson, D. Chandler, D. McQuarrie, S. K. Ma (along with the textbook on Critical Phenomena).*
2. *Chaikin and Lubensky, De Gennes (Scaling Concepts in Polymer), Hansen and McDonald, D. Forster, Boon and Yip.*

CH 512: Chemical Kinetics and Electrochemistry

A. Chemical Kinetics:

- **Condensed Matter:**

1. Rate & Order of Reaction, Determination of Rate Equation, Various types of first order reaction, Principles of Microscopic Reversibility and Detailed Balance, Flow Reactors, Effect of Temperature, Mechanism of Chemical Reactions, Relation between rate constants for the forward and backward reactions, molecularity of a reaction (uni, bi & tri), Unbranched & Branched Chain reaction, Analyses of Complex Reaction Systems and Solution of Coupled Linear Rate Equations.
2. Simple Collision Theory of Bimolecular Reactions, Potential Energy Surfaces, Theoretical Calculations of a Rate Constant, Transition State Theory, Hinselwood's modification, Rice-Ramsperger-Kassel-Marcus Theory (a small touch) Thermodynamic Formulation of TST, Molecular Beam Experiments, Principles of Photochemistry, Rates of Intramolecular Processes, Quenching, Intermolecular processes, Chemical Reactions and their Quantum Yields, Flash Photolysis, Femtosecond Transition State Spectroscopy, Small discussions on Photosynthesis and Photochemical Cell.
3. Kinetics in the Liquid Phase: Rate constants for elementary reactions in water, Acid and Base Catalysis, Kinetic Salt effect, Enzyme Catalysis (Michaelis-Menten Kinetics), Stern-Volmer description, Electrochemical Kinetics; Kinetics of the Hydration of CO2.
4. Solvation as an example of non-reactive dynamics, time scales for solvation in simple liquids and dynamical solvent control on reaction rates. Factors that determine the fast response and its coupling to the environment, time scales found in trapped solvents and solvents (water) near macromolecular surfaces;

Suggested books:

1. *J. I. Steinfeild, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics, Englewood Cliffs, NJ: Prentice Hall, 1989*
2. *R. D. Levine and R. B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity. New York: Oxford Univ. Press, 1987.*
3. *R. B. Bernstein, Chemical Dynamics via Molecular Beam and Laser Techniques. New York: Oxford Univ. Press, 1982.*
4. *I. H. Seagal, Enzyme Kinetics. New York: Wiley-Interscience, 1975.*
5. *R. A. Alberty and R. J. Silbey, Physical Chemistry. John Wiley and Sons*
6. *P. W. Atkins, Physical Chemistry, 5th Edition. ELBS with Oxford Univ. Press.*

7. *A. H. Zewail, Science, volm. 242, 1645 (1988).*
8. *G. R. Fleming and P. G. Wolynes, Phys. Today, volm.43, 36 (1990)*
9. *H. A. Kramers, Physica, volm.7, 284 (1940).*
10. *R. F. Grote & J. T. Hynes, J. Chem. Phys. Volm.73, 2715 (1980).*
11. *M. Maroncelli, J. McInnis, G. R. Fleming, Science, volm.243, 1674, (1989); Jimenez et al., Nature, volm. 369, 471, (1994).*
12. *M. Gavrilla (Ed.), Atoms in Intense Laser Fields, Academic Press*

B. Electrochemistry:

- Equilibrium Aspects:

  Theory of Electrolytic Dissociation: (3L)

  Arrhenius' Theory, Concept of Strong & Weak Electrolytes
  Theory of Ionic Interaction
  Concept of Activity Coefficient & Ionic Strength
  Debye Huckel Theory & Beyond
  Solvation and Hydration of Ions

  Theory of Acids & Bases, Concept of Effective Size of Ions Non-equilibrium Aspects:(5L)

  Electrical Conductance of Electrolytic Solutions
  Conductivity & Conductometric Titrations
  Theory of Electrolytic Conductance
  Debye-Onsager Theory
  Wien Effect
  Abnormal Mobility of Hydrogen and Hydroxide Ions
  Conductance of Nonaqueous Electrolyte Solutions
  Diffusion Phenomena in Electrolytes
  Fick's Law in Electrolyte Solutions

- *Electrode Related Electrochemistry*

  Equilibrium Aspects: (4L)

  Equilibrium Electrode Potentials
  Electrodes of Various kind
  Standard Electrode Potentials & Electrochemical Series
  Electrochemical Cells
  Chemical cells
  Concentration Cells
  Potentiometric Titrations
  Theory of Electrode Potentials
  Nernst Equation & Origin of EMF in Galvanic Cells
  Theory of Electric Double Layer: Models & Thermodynamics
  Electric Double Layer at the Surfaces of Colloids & Micelles

- *Non-equilibrium Phenomena:* (8L)

  Electrolysis
  Faraday's Laws, Electroanalysis
  Kinetics of Electrode Processes
  Concentration Polarization & Overvoltage
  Mechanism of Electrochemical Overpotential

Polarography
Miscellaneous & Modern Kinetic Aspects:

Hydrogen Evolution in Electrolysis
Activated Barrier Crossing Processes in Electrode Processes
Electrodeposition of Metals from Metal Ion Solutions
Electrochemical Dissolution
Electrochemical Corrosion
Fuel Cells
Electron-Transfer Reactions
Marcus Theory & Beyond

Suggested books:

1. *S. Glasstone, An Introduction to Electrochemistry, Litton Educational Publishing, NY.*
2. *J. O'M Bockris & A. K. N. Reddy, Modern Electrochemistry, Plenum Press, NY.*
3. *H. S. Harned and B. B. Owen, The Physical Chemistry of Electrolyte Solutions, 3rd. Edition, Reinhold, NY.*
4. *H. S. Frank, Chemical Physics of Ionic Solutions, Wiley, NY.*
5. *R. A. Robinson and R. H. Stokes, Electrolyte Solutions, 2nd. Ed., Butterworth, London.*

CH 513: Inorganic Chemistry-III

- **Neo-Coordination Chemistry:**
  Macrocyclic chemistry: Macrocyclic effect, template effect-illustrated by acyclic, macrocyclic and macropolycyclic ligand systems, selectivity trends and applications to removal of toxic metals from the environment. Metal promoted chemicals reactions and catalysis.

  Supramolecular chemistry: History, Definition, Biological Inspiration, Intermolecular Interactions, Driving Forces for the Formation of Supramolecular Structures, Hydrogen bonding in Supramolecular Synthesis, Cation-Binding Hosts, Basic Anion coordination chemistry, crown-ethers, cryptands, Cyclophanes.

- **Bioinorganic Chemistry:** Essential chemical elements, metals in biological systems, Dioxygen Carriers: Hb, Mb, Hc, Hr; Copper enzymes: Electron transfer proteins (azurin, plastocyanin); Hydrolytic Enzymes, Zinc and other metal ions; Metals in medicine.

- **Kinetics and Mechanism in Coordination Chemistry**
  Kinetics of substitution reaction in square planar complexes, Trans Effect, kinetics of substitution reaction in octahedral complexes, racemization and isomerization, kinetics of redox reactions, kinetics of electron transfer and photochemical reaction.

Suggested books:

1. *Douglas, McDaniel and Alexander, Concepts and Models of Inorganic Chemistry, 3rd Ed, Wiley, New York, 1994.*
2. *James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity (4th Edition), Publisher: Benjamin Cummings.*

3. *Gary Wulfsberg, Inorganic Chemistry, University Science Books, USA.*
4. *L.F. Lindoy, The Chemistry of Macrocyclic Ligand Complexes, Cambridge, 1989.*
5. *E.C. Constable, Coordination Chemistry of Macrocyclic Compounds, OUP,1999*
6. *J-M. Lehn, Supramolecular Chemistry, VCH, Weinheim, 1995.*
7. *J. W. Steed, J. L. Atwood, Supramolecular Chemistry, John-Wiley and Sons Ltd, 2002.*
8. *Lippard, S.J., Berg, J.M., Principles of Bioinorganic Chemistry, University science Books, CA, 1994.*
9. *Katakis, D., and Gordon, G., Mechanisms of Inorganic Reactions, Wiley, New York, 1987.*
10. *Basolo, F., and Pearson, R.G., Mechanisms of Inorganic Reactions.*
11. *Wilkins, R. G., Kinetics and Mechanism of Reactions of Transition Metal Complexes, 2nd Rev. Edition, VCH, 1991*

CH 514: Organic Chemistry-III

- Energy Surfaces and Kinetic Analyses
    a. Transition state theory and related topics
    b. Postulates and principles related to kinetic analysis, Hammond Postulate, The Curtin-Hammett Principle
    c. Kinetic analyses for simple mechanisms

- Experiments Related to thermodynamics and kinetics
    a. Isotope effect
    b. Substituent effects
    c. Hammett Plots-The most common LFER
    d. Other linear free energy relationships
    e. Acid-Base related effect
    f. Miscellaneous Experiments for Studying Mechanisms

- Catalysis
    a. General principles
    b. Bronsted acid base catalysis
    c. Enzymatic catalysis

Suggested books:

1. *Modern Physical Organic Chemistry - Eric V. Anslyn and Dennis A. Dougherty, University Science Books, 2006.*
2. *Advanced Organic Chemistry, 5th ed. Part A: Structure and Mechanisms – F.A. Carey and R. J. Sundberg, Springer, 2007.*

CH 515: Techniques in Chemistry-II: Molecular Spectroscopy

I. Preliminaries:
Phenomenological treatment of absorption, emission, and scattering. Einstein coefficients, Spectral lineshapes, and Principles of laser emission. Time dependent

perturbation theory, Transition probabilities – Fermi Golden Rule, Finite lifetime of states. (5L)

II. Rotational spectroscopy:
Rigid rotor, Rotational spectra of diatomic molecules, Rotation levels of polyatomic molecules: spherical, symmetric, and asymmetric tops, Angular momentum couplings, Hindered rotations. (5L)

III. Vibrational spectroscopy
Vibration of diatomic molecules, Harmonic and anharmonic oscillator, Vibration of polyatomic molecules. Normal modes and group theory. Vibrational circular dichroism spectroscopy, Fermi interactions, vibrational angular momentum, Coriolis perturbations and inversion doubling. (8L)

IV. Electronic spectroscopy of molecules
Electronic absorption spectra of diatomic molecules. Molecular orbitals and term symbols. Dissociation and pre-dissociation in the spectra of diatomics, Electronic absorption spectra of polyatomic molecules, vibrational structures in electronic spectra, vibronic coupling: Herzberg Teller effect, Jahn-Teller effect, and Renner Teller Effect. Fluorescence. Circular dichroism, Solvent effects. (15L)

V. Introduction to non-linear spectroscopy
Two-photon and higher order processes (4L)

VI. Introduction to the time-dependent approach to spectroscopy
Wavepackets and spectra as Fourier transforms of correlation functions (3L)

Suggested books:

1. *Spectra of Atoms and Molecules - Peter F. Bernath, Oxford University Press*
2. *Modern Spectroscopy - J. M. Hollas, Wiley*
3. *Quantum mechanics in chemistry - G. C. Schatz and M. A. Ratner, Prentice Hall*

COURSE CONTENTS

SECOND YEAR: SEMESTER IV

CH 521: Techniques in Chemistry-III

- Determination of size and shape of molecules*:* X-Ray diffraction, properties of crystals, determination of molecular structure by x-ray crystallography. Transmission Electron microscopy, neutron scattering and light scattering.

- Optical detection of Single molecules and fluorescence correlation spectroscopy: Total internal reflection and confocal optics for single molecule detection (SMD), basic instrumentation for SMD, single molecule photophysics and biochemical

application of SMD. Principle of fluorescence correlation spectroscopy (FCS), basic instrumentation and application to various bio physical processes.

- Scan Probe Microscopy: Atomic force microscopy: Development history, basic principle, image formation mechanism, basic instrumentation, practical aspects of high resolution imaging, sensor applications, soft lithography and fabrication. Scanning tunneling microscopy: Basic principle, instrumentation, imaging application, use in electrochemistry. Tunneling spectroscopy.

- Electron Paramagnetic Resonance (EPR) Spectroscopy: Basic principles, presentation of the spectrum, *g*-value, elementary ideas on hyperfine splitting. Brief discussions on anisotropies in g-factor and hyperfine splitting, EPR of triplet states, Nuclear Quadrupole interaction and line widths. Applications of EPR in determining the geometry of transition metal complexes and biological systems.

- Basic Ideas on Extended X-ray Absorption Fine Structure (EXAFS) and X-ray Absorption Near-edge Structure (XANES).

- Mossbauer Spectroscopy: Isomer shifts, quadrupole interaction, magnetic interaction, applications.

- MCD spectroscopy: Theory of MCS spectroscopy (A, B and C terms, MCD signs, VTVH MCD), Applications of MCD (geometrical structures, electronic structure)

Suggested books:

1. *R. S. Drago, 'Physical Methods for Chemists', Saunders College Publishing*
2. *Inorganic Electronic Structure and Spectroscopy Vol I: Methodology, Ed. By E. I. Solomon, A. B. P. Lever, John-Wiley and Sons, Inc.*
3. *Inorganic Electronic Structure and Spectroscopy Vol II: Applications and Case studies, Ed. By E. I. Solomon, A. B. P. Lever, John-Wiley and Sons, Inc.*
4. *Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism Edited by Lawrence Que, Jr.*
5. *Principles of Fluorescence Spectroscopy- J. R. Lakowicz (Springer)*
6. *Biophysical chemistry part-II: Techniques for the study of biological structure and function- Cantor and Schimmel (Freeman).*
7. *Transmission electron microscopy- D. B. Williams and C. B. Carter (springer)*
8. *Scanning Probe Microscopy and Spectroscopy: Theory, Techniques and applications- D. A. Bonnell (Wiley-Vch)*

CH 522: Elective-I

I. Time Dependent Quantum Mechanics and Chemical Dynamics

Second Quantization: Applications of Second Quantization, The Linearly Forced Harmonic Oscillator, Coherent States, Energy Transfer in Polyatomic Molecules, Energy Transfer to Solids.

Effective Hamiltonian Approaches: Gaussian Wavepackets, The Classical Path Equations, Correction to the SCF Approach, Wave Operator Approach.

Semiclassical Theories: Feynman Path Integrals, The Short - Time Propagator, The Classical Limits, Semiclassical Feynman Path Theory, Classical S – Matrix Theory, Resolution in Eigenstates and Statistical Mechanics.

Wavepacket Propagation: Fourier Transform Method, DVR Method, Time Propagation, Bohm Trajectories, Tunneling of Wavepackets, Absorbing Boundaries.

The Born – Oppenheimer Treatment: The Born – Oppenheimer Treatment, The Non – Adiabatic Coupling Terms and the Adiabatic Representation, The Diabatic Representation, Discussion – A Comparison Between the Two Frameworks, The Adiabatic – Diabatic Transformation, The Adiabatic – Diabatic Transformation Matrix A, Solutions of the First Order Equation in an N Dimensional Hilbert Space, Solutions of the First Order Equation in a Two Dimensional Hilbert Space, The Jahn – Teller Model, The Longuet – Higgins Phase and the Berry Phase, The Extended Born – Oppenheimer Equation.

Reaction Dynamics: Various Coordinate Systems - The Atom Tri – Atom System, The Collinear Arrangement, Minimum Energy Path, A Model Study (Quantum Mechanical Treatment), Resonance, Time Delay, The Reaction Coordinates, Stark – Werner Potential.

Suggested books:

1. *G. D. Billing, K. V. Mikkelsen 'Advanced Molecular Dynamics and Chemical Kinetics ', John Wiley and Sons Ltd*
2. *M. Baer, Beyond Born-Oppenheimer: Electronic Nonadiabatic Coupling Terms and Conical Intersections, John Wiley and Sons Ltd*
3. *George C. Schatz, Introduction to Quantum Mechanics in Chemistry, Prentice Hall*

II. Advanced Quantum Mechanics

1. Some Phenomena in Quntum Mechanics
   a. Double Slit experiments
   b. Linear vector space and linear operators ,self adjoint operators, Hilbert space and rigged Hilbert space, Probability Theory
   c. The formulation of Quantum Mechanics, Basic Theoretical concepts, conditions on operators, general states and pure states, probability distributions
   d. Kinematics and dynamics, Transformation of states and observables, the symmetries of space- time, Generators of Galeli Group, operators and dynamical variables, equation of motion and conservation laws
2. Coordinate representation and applications:
   Galelei transformation of Schrodinger equation,
   probability flux, conditions on wave functions,
   tunneling, path integrals
3. Momentum Representation and applications:
   Momentum distribution in atoms,Bloch's Theorem,
   Diffraction Scattering: Theory and Experiment

4. Angular momentum-orbital motion and spin, discrete symmetries, space inversion and time reversal, parity non-conservation, Permutation symmetry and many particle systems, Hartree Fock equation and beyond, PT-symmetry
5. Charged particle in a magnetic field :Classical and Quantum theory, motion in a static Uniform magnetic field, The Aharonov-Bohm effect, The Zeeman Effect, Quantum Mechanics of electromagnetic field
6. The Classical Limit :Quantum Mechanics in Phase space, The Wigner and Husimi Distributions
7. Relativistic Quantum Mechanics, Klein Gordon and Dirac equations, Applications, Dirac Hartree Fock Method
8. Supersymmetric Quantum Mechanics : Simple Applications

Suggested books:

1. *L E Ballentine, Quantum Mechanics: A Modern Development, world scientific*
2. *Franz Schwabl, Quantum Mechanics, Springer Verlag, 2007*
3. *Lev Davidovich Landau, E. M. Lifshitz, Quantum mechanics: non-relativistic theory, Elsevier*
4. *Albert Messiah, Quantum mechanic, Dover Publication*

III. Advanced Statistical Mechanics

- Interacting Classical Systems
- Interacting Bose Systems
- Interacting Fermi Systems
- Phase transition beyond mean field
- Polymer physics and other applications
- Boltzmann transport equation and its applications, calculation of transport coefficients
- Correlation function and linear response theory

Suggested books:

1. *Kerson Huang, Statistical Mechanics, Wiley*
2. *R.K. Pathria, Statistical Mechanics, Butterworth-Heinemann*
3. *Pierre-Gilles de Gennes, Scaling concepts in polymer physics, Cornell University Press*
4. *Michael Plischke, Birger Bergersen, Equilibrium statistical physics, world scientific*

CH 523: Elective-II

I. Advanced Bioinorganic Chemistry

Detailed reaction mechanisms (kinetics and spectroscopic characterization of reaction intermediates) of some biological processes: O_2 reduction by Cytochrome c oxidase and multi copper oxidases (e.g.Laccase); Nitrate to Nitrogen conversion in the bacterial denitrification cycle.

Fe uptake, regulation and storage in the human body
Oxidases vs. Oxygenases (some specific examples), O_2 Activation, Hydroxylation: MMO, P-450, R2
Photosystem-II, Cu-Zn superoxide dismutase,
Bioinorganic Modeling.

Suggested books:

1. *Bioinorganic Chemistry: A Survey, by Eiichiro Ochiai, Elsevier*
2. *Biological Inorganic Chemistry: Structure and Reactivity, by Bertini, Gray, Stiefel and Valentine, University Science Books, USA.*
3. *Principles of Bioinorganic Chemistry, by Stephen J. Lippard and Jeremy M. Berg, University Science Books, USA*
4. *The Biological Chemistry of the Elements, by J. J. R. Frausto da Silva and R. J. P. Williams, 2nd Edition, Oxford University Press*

II. Supramolecular Chemistry and Crystal Engineering

Supramolecular Chemistry

- Host-guest chemistry of Calixarenes, Dendrimers and Cyclodextrins,
- Anion Coordination Chemistry
- Supramolecular assembly in inorganic helical complexes, Catenanes, Rotaxanes, Knots and other Molecules with Interesting Topology like Molecular tweezers, and transition metal-based cationic molecular boxes, second-sphere coordination and catalysis.
- Applications of Supramolecular Chemistry in Chemical Sensing of Ions, Molecular devices, Molecular Machines.

Crystal Engineering

- Organic crystal engineering: Crystal structure from molecular structure, Intermolecular interactions and crystal packing, Supramolecular synthetic strategies, Functionalized solids, Polymorphism,
- Inorganic crystal engineering: Coordination polymer vs Metal-Organic Frameworks (MOFs), Synthetic routes to MOFs, Secondary building unit (SBU) concept, Potential applications of MOFs (gas storage, separation, magnetism, drug delivery, etc.)

Suggested books:

1. *J-M. Lehn, Supramolecular Chemistry, VCH, Weinheim, 1995.*
2. *J. W. Steed, J. L. Atwood, Supramolecular Chemistry, John-Wiley and Sons Ltd, 2002.*
3. *Kristin Bowman-James, Antonio Bianchi, Enrique Garcia-Espana, Anion Coordination Chemistry; Wiley-VCH Verlag, 2011.*

CH 524: Elective-III

I. Advanced Organic Synthesis

Logic of synthesis; retrosynthesis; 'atom economy'

Carbon-carbon and carbon-hetero atom bond formation; main group and transition metals as reagents; chemo-, regio- and stereoselectivity

Modern aldol reaction in the context of macrolide synthesis

Ring-forming reactions; synthesis of medium-size rings; linearly fused and angularly fused ring-systems

Transition metal-mediated ring synthesis; reactions of metal-coordinated polyene and polyenyl ligands; higher-order cycloadditions

Aromatic and heterocyclic synthesis; directed metalation; heterocycles as latent synthons

Metal - catalyzed hydrogenation, hydrosilylation and hydroformylation; hydrozirconation; conjugate addition; alkene and alkyne metathesis; enantioselective catalysis by chiral Lewis acids

Oxidation and reduction; chemoselectivity; enantioselectivity

Suggested books:

1. *Advanced Organic Chemistry Part B – F. A. Carey and R. J. Sundberg, 5th Ed, Springer, 2007.*
2. *The Logic of Organic Synthesis – E. J. Corey and X.-M. Cheng, Wiley, 1995.*
3. *Classics in Total Synthesis – K. C. Nicolaou and E. J. Sorensen, Wiley-VCH, 1996.*
4. *Classics in Total Synthesis – K. C. Nicolaou and S. A. Snyder, Wiley-VCH, 2003.*
5. *Transition Metals in the Synthesis of Complex Molecules – L. S. Hegedus and B. C. G. Soderberg, 3rd Ed, University Science Books, 2009.*
6. *Organic Synthesis: The Disconnection Approach – S. Warren and P. Wyatt, 2nd Ed, Wiley, 2009.*
7. *Organic Synthesis: Strategy and Control – P. Wyatt and S. Warren, Wiley, 2007.*

II: Stereoselective Synthesis

Chirality in nature – molecular and supramolecular chirality – utility of chiral organic molecules – forms of chirality – asymmetric carbon – axial chirality – planar chirality – analytical methods for optical isomer separation and identification – determination of optical purity – resolution of optical antipodes – chiral HPLC

Diastereoselective synthesis; Prelog's rule and chiral auxiliary approach; chirally modified reagents; TADDOL; use of 'chirons' and chiral pool
Cram's rule and beyond; chelation-control and non-chelation-control; chiral amplification in organozinc addition; non-linear effects in asymmetric synthesis

Asymmetric aldol reaction; enolates of lithium, boron, tin, titanium, zinc, etc. – configuration of enolates and stereochemistry of aldehyde addition – product assignment and extent of stereocontrol – transition state models; 'double stereodifferentiation' as a concept; popular and generally adaptable chiral auxiliaries (Oppolzer, Evans, Enders, Davies, 8-phenyl-menthol, BINOL, etc.)
Asymmetric hydroboration; boronic ester homologation; enantioselective deprotonation and protonation; alkylation of chiral nucleophiles; Meyer's oxazoline based nucleophiles; 'memory of chirality'
Asymmetric catalysis; asymmetric carbometalation; asymmetric carbene addition and insertion; asymmetric cycloaddition and ene reaction; asymmetric cross-coupling reactions; asymmetric phase-transfer catalysis; autocatalysis
Asymmetric organocatalysis; enzymatic catalysis

Suggested books:

1. *Principles of Asymmetric Synthesis – R. E. Gawley and J. Aub, Pergamon, 1996.*
2. *Catalytic Asymmetric Synthesis, 3rd Ed - I. Ojima(ed.), Wiley, 2010.*
3. *Asymmetric Catalysis in Organic Synthesis – R. Noyori, Wiley, 1994.*
4. *Asymmetric Synthesis, vol 1-5 – H. S. Mosher and J. D. Morrison(ed.), Academic Press.*
5. *Classics in Stereoselective Synthesis – E. M. Carreira and L. Kvaerno, Wiley-VCH, 2008.*
6. *Asymmetric Synthesis : The Essentials -, M. Christmann and S. Bräse (ed.), Wiley-VCH, 2007.*
7. *Asymmetric Synthesis with Chemical and Biological Methods – D. Enders and K. –E. Jaeger, Wiley-VCH, 2007.*

III: Bio-Organic and Medicinal Chemistry

Common mechanisms in biological chemistry

Biomolecules; synthesis of peptides and oligonucleotides; polysaccharides

Enzyme chemistry; coenzymes and cofactors; metal ions in bio-catalysis; substituted and beta-amino acids for peptide mimetics

Molecular recognition in biology; self-assembly; synthetic receptors; PNAs and anti-sense research; molecular communication between cells

Lipid metabolism; carbohydrate metabolism; amino acid metabolism; nucleotide metabolism

Biosynthesis of some natural products; bio-mimetic synthesis

Biological transformations; industrial applications

Mechanism-based drug design; competitive inhibitors and suicide substrates; natural products as 'lead' structures; antibiotics and drug resistance; biofilm; target-specific drug-delivery; challenge of ageing

Suggested books:

1. *An Introduction to Medicinal Chemistry – G. L. Patrick, OUP, 2009.*
2. *Molecules and Medicines – E. J. Corey, L. Kuerti and B. Czako, Wiley, 2007.*
3. *The Organic Chemistry of Drug Design and Drug Action – R. Silverman, Academic Press, 2004.*
4. *The Organic Chemistry of Biological Pathways – J. McMurry and T. Begley, Roberts and Company Publishers, 2005.*
5. *Medicinal Natural Products: A Biosynthetic Approach – P. M. Dewick, Wiley, 2009.*
6. *The Biosynthesis of Natural Products: An Introduction – J. D. Bulock, McGraw-Hill, 1965.*

IV: Asymmetric Synthesis and Catalysis

Introduction – Scope of the study

Chirality in nature – molecular and supramolecular chirality – utility of chiral organic molecules – forms of chirality – asymmetric carbon – axial chirality – planar chirality – analytical methods for optical isomer separation and identification – determination of optical purity – resolution of optical antipodes – chiral HPLC

Chiral induction – Diastereoselective synthesis

Stereoselectivity and stereospecificity – 1,2-induction and 1,3-induction – Cram's rule and beyond – chelation-control and non-chelation-control – directed functionalization – directed biomimetic polyene cyclization (Johnson)

Chiral Pool approach – Diastereoselective Synthesis

'Chirons' – terpenes and carbohydrates as chiral source material – Steven's steroid intermediate synthesis – alkaloid synthesis – limitations

Chiral auxiliary – Diastereoselective synthesis

Basic requirements of a chiral auxiliary – 'chiral pool' sources – popular and generally adaptable chiral auxiliaries (Oppolzer, Evans, Enders, Davies, 8-phenyl-menthol, BINOL, etc.) – kinetic resolution by chiral auxiliary – boronic ester mediated homologation – disadvantages of 'auxiliary' approach

Asymmetric aldol condensation and Alkylations

Equilibrium-controlled condensation reaction has its own disadvantages – transition state – enolates of lithium, boron, tin, titanium, zinc, etc. – configuration of enolates and stereochemistry of aldehyde addition – product assignment and extent of stereocontrol – transition state models – 'double stereodifferentiation' concept – Masamune's sugar synthesis – macrolide antibiotics as target – alkylation of chiral nucleophiles – Meyer's oxazoline based enolates, Evan's oxazolidinone derived enolates – polyanions in peptide backbone (Seebach)

Chirally modified reagents

Reducing agents like boron/aluminium hydrides – allylation and crotylation – oxazaborilidines – TADDOL – chiral lithium amides – chiral Lewis acids in enolate reactions, cycloadditions and sigmatropic rearrangements –

enantioselective deprotonation and protonation – "chiral cavity" for enentioselection

Asymmetric catalysis

Metal mediated catalysis – biocatalysis – organocatalysis – 'non-linear effects' – 'ligand accelerated catalysis' and 'chiral amplification'.

Suggested books:

1. *Catalytic Asymmetric Synthesis, 3rd Ed - I. Ojima(ed.), Wiley, 2010.*
2. *Asymmetric Catalysis in Organic Synthesis – R. Noyori, Wiley, 1994.*
3. *Asymmetric Synthesis, vol 1-5 – H. S. Mosher and J. D. Morrison(ed.), Academic Press.*
4. *Asymmetric Synthesis : The Essentials -, M. Christmann and S. Bräse (ed.), Wiley-VCH, 2007.*
5. *Asymmetric Synthesis with Chemical and Biological Methods – D. Enders and K. –E. Jaeger, Wiley-VCH, 2007.*
6. *Comprehensive Asymmetric Catalysis, I-III – E. N. Jacobsen, A. Pfaltz and H. Yamamoto, Springer, 1999.*

V: <u>Chemistry and Biology of Natural Products</u>

Synthesis of biologically and medicinally important natural products.

Chemical library synthesis of the useful natural products using solid supported synthesis and diversity oriented synthesis (DOS).

Mode of action in biological pathway.

Derive most potent drug from the natural product skeleton.

Case studies:

Suggested books:

1. *Natural Products Drug Discovery and Therapeutic Medicine edited by Lixin Zhang and Arnold L. Demain (humana Press)*
2. *Chemical Biology (Small Molecules to System Biology and Drug Discovery) edited byStuart Schreiber and Tarun kapoor*
3. *The Logic of Chemical Synthesis by E. J. Corey and X-M Cheng.*
4. *Classics in Total Synthesis by K. C. Nicolaou and E. J. Sorensen.*
5. *Current opinion in chemical biology, 2005, 9, 248. (by Shiying Shang and Derek S Tan).*
6. *Nature reviews, 2005, 4, 35 (by Leonard I. Zon and Randall T. Peterson).*
7. *Stuart L. Schreiber (publication lists from Harvard University, Chemical Biology).*
8. *Diversity-based organic synthesis in the era of genomics and proteomics by Prabhat Arya, Angew. Chem. Int. Ed. Engl. 2001, 40/2, 339.*

<u>CH 525: Elective-IV</u>

I. <u>Advanced Macromolecular Chemistry</u>

Controlled ("living") polymerization- (ATRP, RAFT, NMP), mechanism and kinetics.
Block copolymers: Synthesis and characterization
Conducting polymers: Synthesis, photophysical properties, applications (organic optoelectronics- LED, photovoltaic).
Amphiphilic polymers in solution: Structural variations in amphiphilic polymers, aggregation properties in aqueous solution, thermodynamics and kinetics of various aggregation process, encapsulation, stimuli-sensitive assemblies, implications in drug-delivery.
Interaction of synthetic polymers with bio-macromolecules: Polymer-protein interaction, polymer-DAN interaction, enzyme inhibition, gene delivery etc.
Helical polymers: Foldamers, rigid helical polymers, structural and functional aspects of bio-mimicking.
Supramolecular polymers: Various molecular designs, gels, assemblies.
Liquid crystalline polymers: Structure and function

Suggested books:

1. *Principles of Polymerization: George Odian*
2. *Block Copolymers in Solution (Ed: I. W. Hamely)*
3. *Molecular Recognition and Polymers (Ed: V. Rotello)*
4. *Foldamers(Ed: I. Huc)*
5. *Nano-structured Conductive Polymers (Ed: A. Eftekhari)*

II. Advanced Materials Science

- Surface science
- Solid-Solid interfaces
- Nanomaterials and properties

III. Cell Biology

Basic functions of cells (5), Biomolecules (2), Central Dogma (3), regulation of replication, transcription and translation (15), Bio-physics (15):

Suggested books:

Biochemistry: (a) Lehninger, Nelson, Cox; (b)Voet, Voet; Stryer

Biophysical Chemistry: (a) Cantor, Schimmel; (b)Tinoco, Wang; (c)van Holde

Molecular Biology of the Cell: (a) Baltimore, Lodish, Darnell; (b) Alberts

Genetics: (a) Suzuki; (b) Russell; (c) Gardener; (d) T.A.Brown

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