

Post-Graduate Catalog

DEPARTMENT OF CHEMISTRY

School of Natural Sciences

SHIV NADAR UNIVERSITY



About Chemistry Department (<https://chemistry.snu.edu.in/>)

Chemistry education at SNU provides a link between the fundamental principles governing the nature of the universe and the science of life, and spans traditional as well as a variety of inter-disciplinary areas. Chemistry, often referred as the central science, as it plays a vital role in nearly every other scientific field.

The Department is committed in pursuing research on fundamental and applied problems through scientific inquiry, and to stimulate the development of innovative interdisciplinary research programs around key areas of excellence. The immediate mission of Chemistry Department is to:

- Contribute to the advancement and dissemination of chemistry knowledge through educational programs, high quality publications in peer-reviewed international journals and innovative patents.
- Devise robust and novel solutions to address the needs of society by promoting research into chemical and interdisciplinary projects.
- Train undergraduate, graduate students and research fellows to generate future independent scientists to serve the needs of society, academia and industries.

Our vision is to make our world a better place through societal-impact cutting-edge research and innovation at Shiv Nadar University.

Post-Graduate Programs

At the postgraduate level, we offer Integrated B.Sc.-M.Sc.-Ph.D. with Integrated B.Sc.-M.Sc. (Research) as an exit option, Integrated M.Sc.-Ph.D. with M.Sc. (Research) as an exit option, and Ph.D. There are multiple options for achieving various degrees depending on the student's choice, if they maintain the required CGPA. In a normal scenario, one can obtain Integrated B.Sc.-M.Sc. (Research) degree for 5 years, Integrated B.Sc.-M.Sc.-Ph.D. for 8 years, Integrated M.Sc.-Ph.D. for 5 years, M.Sc. (Research) for 2 years and Ph.D. for 4 years.

Post-Graduate Courses

Chemistry PG courses are designed in such a fashion that allows the students to develop their knowledge further on both the fundamentals of chemistry viz. organic, inorganic, physical and analytical chemistry and simultaneously correlate the knowledge gained at the various probable interfaces. The knowledge acquired is further strengthened with the computational aspects, and related applications, wherever possible. A vast opportunity to choose a varied set of elective courses in the curriculum allow students to prepare for their future opportunities. Foundation courses in the first semester ensure that all students possess the requisite background to complete the course of study

and benefit fully from the program. Well-equipped research labs offer good platform to the students to learn and improve the research skills, develop capabilities to write research proposals, research exposure via in-depth dissertation under the supervision of a research advisor, and enhance capability to present scientifically during the course structure. This includes literature seminars, presentation skills and more importantly a public thesis defense. The chemistry department offers a flexible and broad curriculum that prepares students in a step-wise manner not just for a career in chemistry and related fields upon graduation, but also assists in acquiring the leadership qualities.

Eligibility for Post-Graduate Programs

While students with 60% in M.Sc. in natural sciences are eligible to apply for the Ph.D. program, the students with CGPA equivalent to 60% marks in B.Sc. (3 years) in chemistry are eligible to apply for the integrated M.Sc.-Ph.D. and M.Sc. (Research) programs. Major courses in the first two semesters ensure that the students possess and attains both the basic and advance further in all the requisite courses including inorganic, organic and physical chemistry. A key goal of the post-graduate programs is to offer innovative thinking skills to the students. And by preparing them with both the essential and advance skills required to have better prospects in future. This preparedness is essential not only in terms of developing a sustainable world but also adaptability to the ever-changing job-market. This is achievable together with our outstanding faculty of international repute education.

Chemistry Careers

Chemistry at SNU offers good career opportunities for Ph.D., post-doctoral fellowship, jobs in industry as well as in academia, within India and abroad such as US, Europe, Japan and Australia and others. The major employers being: industries related to agricultural technology, biotechnology, pharmaceuticals, materials and related applications. Furthermore, chemists may find job opportunities in various other sectors such as chemical industry, and advancement of career opportunities in forensic, food science and as health professionals.

Chemistry Research at SNU

Research activities are not confined to post-graduate level, but are integrated with the undergraduate program at SNU through various lab-related components and possibility using Research Experiential & Applied Learning (REAL) course platform too. Undergraduate research allows students to realize and reinforce chemistry knowledge from their formal course work. It also assists in developing their scientific and professional skills, and create acumen towards answering out of the box questions. Original research culminating in a comprehensive written report provides an effective pedagogical means for integrating undergraduate learning experiences, and allows students to participate directly in the learning process.

Opportunities for research in chemistry at SNU are available in the following broad areas:

- Catalysis
- Chemical Biology
- Cheminformatics
- Computational Quantum Chemistry
- Crystallography
- Green Chemistry
- Materials Chemistry
- Medicinal Chemistry
- Metalloradical Chemistry
- Protein Chemistry
- Supramolecular Chemistry
- Synthetic Organic Chemistry
- Ultrafast Spectroscopy

For specific research areas, please visit here: <https://chemistry.snu.edu.in/research/areas-research>.

Major in Post-Graduate Chemistry

Chemistry department at SNU provides the following post-graduate chemistry courses to link the relation between the fundamental principles of chemistry, inter-disciplinary sciences and its application at the research level. Every chemistry postgraduate student of the University is required to complete a number of credits from various courses as classified into the following categories:

The credit requirements for **M.Sc. (Research) in Chemistry** are:

- **83 credits** = 33 credits in Core Chemistry Courses (Core + Specialized) + 24 credits (Chemistry electives courses) + 24 credits (Master project) + 2 credits Seminar

The credit requirements for **Integrated B.Sc.-M.Sc. (Research) in Chemistry** are:

- **211 credits** = 128 credits from 3 years B.Sc. + 83 credits from 2 years M.Sc.
- 128 credits = 68 credits in Core Chemistry Courses (Introductory + Foundation + In-depth) + 21 credits (courses from Physics/Mathematics/Life Sciences) + 3 credits (Chemistry electives courses) + and 42 credits (18 credits core common curriculum (CCC) courses + 18 credits University Wide Elective (UWE) courses)

The credit requirements for **Integrated B.Sc.-M.Sc.-Ph.D. in Chemistry** are:

- **211 credits** = 128 credits from 3 years B.Sc. and 83 credits from 2 years M.Sc.
- 128 credits = 68 credits in Core Chemistry Courses (Introductory + Foundation + In-depth) + 21 credits (courses from Physics/Mathematics/Life Sciences) + 3 credits (Chemistry electives courses) + and 42 credits (18 credits CCC courses + 18 credits UWE courses)
- 83 credits = 33 credits in Core Chemistry Courses (Core + Specialized) + 24 credits (Chemistry electives courses) + 24 credits (Master project) + 2 credits Seminar

The credit requirements for **Integrated M.Sc.-Ph.D. in Chemistry** are:

- **83 credits** = 33 credits in Core Chemistry Courses (Core + Specialized) + 24 credits (Chemistry electives courses) + 24 credits (Master project) + 2 credits Seminar

The credit requirements for **Ph.D. in Chemistry** are:

- **12 Credits** (includes 6 credit core courses + 6 credit electives courses)

Major courses in Post-graduate Chemistry

Semester	Course	Course Title	L : T : P	Credits
1 (MSN)	CHY512	Advanced Molecular Spectroscopy*	3:0:0	3
	CHY527	Organic Reaction Mechanisms -1	2:1:1***	4
	CHY615	Graduate Seminar*	1:0:0	1
	CHY649	Analytical Chemistry	3:0:1**	4
	CHYxxx	Electives	X:X:X	3
	CHYxxx	Electives	X:X:X	3
	CHY597	Master Project	0:0:6	6
1 (MSN): Total credits: 24				
2 (SPR)	CHY502	Synthetic Organic Chemistry	3:0:0	3
	CHY518	Thermodynamics & Reaction Dynamics	3:0:1***	4
	CHY548	Frontiers in Inorganic Chemistry	3:0:1***	4
	CHY600	Research Methodology*	2:0:0	2
	CHYxxx	Electives	X:X:X	3
	CHYxxx	Electives	X:X:X	3
	CHY598	Master Project	0:0:6	6
2 (SPR): Total credits: 25				
3 (MSN)	CHY547	Chemistry of F-block Elements	3:0:0	3
	CHY619	Advanced Quantum Chemistry	3:0:0	3
	CHYxxx	Electives	X:X:X	3
	CHYxxx	Electives	X:X:X	3
	CHYxxx	Electives	X:X:X	3
	CHY697	Master Project	0:0:6	6
3 (MSN): Total credits: 21				
4 (SPR)	CHY644	Chemistry of Materials	3:0:0	3
	CHY899	Seminar*	1:0:0	1
	CHY6xx	Electives	X:X:X	3
	CHY698	Master Project	0:0:6	6
4 (SPR): Total credits: 13				
Total Credits				83

*Compulsory for Ph.D., ** Practical of 2 hours, *** Practical of 3 hours.

Elective courses:

Course Code	COURSE NAME	L:T: P	Credits
CHY501	Medicinal Chemistry of Organic Molecules(need to update)	3:0:0	3
CHY502	Synthetic organic Chemistry	3:0:0	3
CHY311/511	Chemical Binding ^{##}	3:0:1 ^{***}	4
CHY522	Informatics and Drug Discovery (need to update)	3:0:0	3
CHY526	Chemistry of Natural Products	3:0:0	3
CHY542	Supramolecular Chemistry	3:0:0	3
CHY544	Nanotechnology and Nanomaterials	3:0:0	3
CHY545	Fundamentals of Crystallography	2:0:1 ^{**}	3
CHY552	Polymer Chemistry and its Scope	3:0:0	3
CHY553	Co-ordination and Bio-inorganic Chemistry	3:0:0	3
CHY 554	Green chemistry and Sustainability	3:0:0	3
CHY556	Inorganic reaction mechanism	3:0:0	3
CHY557	Intelligent materials for nanomedicine	3:0:0	3
CHY558	Organometallic Chemistry	3:0:0	3
CHY 601	Quantitative Methods	1:0:0	1
CHY609	Strategies for problem solving	2:0:0	2
CHY611	LASER spectroscopy	3:0:0	3
CHY616	Statistical Mechanics	3:0:0	3
CHY621	Organic Named Reactions II	3:0:0	3
CHY627	Organic Reaction Mechanisms –II	3:0:0	3
CHY352/652	Advanced Biochemistry	3:0:0	3

** Practical of 2 hours; *** Practical 3 hours, ## Compulsory for M.Sc. (Research) or Integrated M.Sc.-Ph.D.

CHY 501: Medicinal Chemistry of Organic Molecules (L : T : P = 3 : 0 : 0)

Every student will present a current paper of his or her choice that focuses on medicinal chemistry. Papers will be suggested but not limited to these suggestions. Each presentation will be roughly 20 minutes. Every presenter needs to prepare at least three questions to start in class discussion (10 minutes) after the presentation. The presenter will be graded on the quality of these questions as well as the ability to address them. The peers will be graded based on the ability to answer my and the presenter's questions. The presentations should be turned in at least one week in advance. Presentations will be 15 min with 5 min for questions. These presentations will be graded based on content, clarity, slide quality, knowledge of the materials, and proper use of the presentation time and the performance during Q&A sessions.

Course Content:

- a) Introduction to Medicinal Chemistry, History
- b) Drug Discovery process
- c) Receptors as targets and drug-target interactions
- d) Metabolism and pharmaceutical properties
- e) Determining target structure
- f) Lead discovery/ lead optimization
- g) Drug Development Process
- h) Week 14: Drug Targets
- i) Student Presentation

CHY 502: Synthetic Organic Chemistry (L : T : P = 3 : 0 : 0) (Major Course)

Students will learn several mechanisms and their applicability, limitations of the major reactions in organic synthesis and especially stereo chemical control in synthesis. Furthermore, recent highlights of new synthetic reactions and catalysts for efficient organic synthesis. Mechanistic details as well as future possibilities will be discussed. Tactics of organic synthesis, planning logic of synthesis and methodology will be learnt. A dissection of the most important syntheses of complex natural and unnatural products and biogenesis will also be discussed.

Course content

Tactics of organic Synthesis	A dissection of the most important syntheses of complex natural and unnatural products. Synthesis, planning and methodology. The logic of synthesis and Biogenesis
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Metal mediated C-C bond formation	Name reactions and mechanism, Applications and limitations of the major reactions in organic synthesis. Application in natural product synthesis and Literature review
New chemistry	Cross-dehydrogenative coupling reactions, C-H bond activation through directing groups. Hypervalent iodine in organic transformation
Olefination reactions	Name reactions and mechanism, Applications and limitations of the major reactions in organic synthesis. Application ion natural product synthesis and Literature review
Organic synthesis in drug discovery	Overview, Small molecules as drugs. Natural products as drugs

CHY311/511: Chemical Binding## (L : T : P = 3 : 0 : 1) (Elective Course for outside SNU)

The course is a basic survey of modern quantum theories chemical bonding from both theoretical and computational standpoints. The course aims at a conceptual understanding of the basic principles of chemical bonding and molecular quantum mechanics. No rote memorization is required or expected. The lab portion of the course aims to equip students to set up, perform and analyze the most common kinds of quantum chemistry and electronic structure calculations with Gaussian basis sets.

Course content

- Theorems of Linear Algebra
- Postulates of Quantum Mechanics
- Atomic Orbitals and Basis Sets
- Born-Oppenheimer approximation and the molecular Hamiltonian
- The Concept of the Potential Energy Surface
- Geometry Optimization and Frequency Analysis
- Semi-empirical and *ab initio* Quantum Mechanics
- Variation and Perturbation Theory
- Spin, statistics and the Pauli principle
- Valence Bond and Molecular Orbital theories
- Independent-Particle Models: the Hartree method

- The Hartree-Fock Self-Consistent Field equations
- Electron Correlation, Density Matrices and Natural Orbitals
- Density Functional Theory
- Atoms in Molecules
- Periodic systems
- Implicit and explicit solvent methods

CHY512: **Advanced Molecular Spectroscopy (L : T : P = 3 : 0 : 0) (Major Course)**

Various state-of-the-art spectroscopy techniques underpin a broad range of research in the field of chemistry, physics and biology. In this course, the principle of quantum mechanics will be introduced to understand series of molecular energy levels and various spectroscopic transitions. A comprehensive theory and application of rotational spectroscopy, infrared spectroscopy, Raman, uv-visible spectroscopy, fluorescence, nuclear magnetic resonance spectroscopy will be taught. In addition, this course also includes role of molecular symmetry and group theory in chemical structure, bonding and reactivity. An emphasis will be provided in designing experiment and interpreting spectra to address chemical research problem relevant to selectivity, reactivity and kinetics. This course will cover how these techniques can be used in basic science for understanding chemical structure and composition, electronic structure and interaction of chemical compounds.

Course content

Group theory	Time-independent and time-dependent perturbation theory, Discrete and continuous groups, Group multiplication tables, Generators, Symmetry elements, Symmetry operations and point groups, Reducible and irreducible representations, The Great Orthogonality Theorem and character tables, Projection operators and symmetry-adapted linear combinations (SALCs), Spectroscopic selection rules.
Rotational spectroscopy	Introduction and review, Rotational spectroscopy of diatomic rigid and non-rigid molecules, Polyatomic linear and symmetric top molecules.
Vibrational spectroscopy	Energy of harmonic oscillator, Morse potential and anharmonic oscillator, Vibrational selection rule, Infrared spectroscopy, Vibrating rotator,

(Infrared)	Breakdown of Born-Oppenheimer approximation, Birge-Sponer plot, Vibration of polyatomic molecules, Normal modes.
Vibrational spectroscopy (Raman Scattering):	Classical and quantum pictures of light scattering, Classical theory of Raman spectroscopy, polarizability and polarizability tensor, Rotational Raman spectra, Vibrational Raman spectra, Rule of mutual exclusion.
UV-vis spectroscopy	Theory of UV-Vis spectroscopy, Lambert-Beer's Law, Born-Oppenheimer Approximation and molecular potential energy curve, Molecular term symbol, Franck-Condon principle, Selection rule, transition moment, intensity of electronic spectra and Franck-Condon factor, Spin-orbit coupling.
Fluorescence spectroscopy	Primary photochemical process, Jablonski diagram, Fluorescence and phosphorescence, Vibrational relaxation, Non-radiative and radiative processes, Internal conversion and Intersystem crossing, Stokes Shift, Effect of solvent on Stoke shift, Decay of excited state, fluorescence lifetime and quantum yield, Fluorescence quenching and Stern-Volmer equation, Static and dynamic quenching.
Nuclear Magnetic Resonance (NMR)	Nuclear spin, Spin angular momentum and its quantization, Nuclear magnetic moment, Interaction between nuclear spin and external magnetic field, Larmor precession, Sensitivity of NMR, Chemical shift, Origin of shielding constant, Anisotropic effect, Theory of spin-spin coupling for first order (perturbation theory) and second order (variational method) spectra, Pulse techniques in NMR, Rotating frame of reference, $\pi/2$ and π pulses, Spin-spin relaxation and spin-lattice relaxation, Fourier Transform NMR, Nuclear Overhauser effect (NOE), Concept of 2-dimensional NMR spectroscopy, 2D-Correlation spectroscopy (2D COSY), 2D-Nuclear Overhauser Effect spectroscopy (2D NOESY).

CHY518: Thermodynamics & Reaction dynamics (L : T : P = 3 : 0 : 1) (Major Course)

Chemical reaction dynamics provides the most fundamental insight of chemical reaction as it deals with the motion of constituent atoms in reacting molecules. Both theoretical and experimental studies provide the detailed mechanism of time evolution of chemical reaction at molecular level. In this course, various techniques for studying very fast reactions, basic statistical mechanics,

thermodynamical and statistical formulation of transition state theory, theories of gas phase and solution phase reactions, potential energy surface, enhancement of reaction rate and different experimental studies of chemical reactions dynamics including crossed molecular beam experiment, state-to-state kinetics and study of transition state species will be discussed. Course will cover the connection between macroscopic chemical kinetics and microscopic reaction dynamics. Moreover, some of the advanced topics of electrochemistry will also be covered in the course.

Course content

Thermodynamics	Nernst heat theorem, Third law of thermodynamics, phase cell, microcanonical, canonical and grand canonical ensembles, Thermodynamical probability and entropy, Maxwell-Boltzmann statistics, molecular partition functions, translational, rotational, vibrational and electronic contribution to the partition function.
Electrochemistry	Mean ionic activity co-efficient, Debye-Huckel theory of ion-ion interaction, Poisson's equation, modification and extension of Debye Huckel theory to concentrated solution, ion association, Debye-Huckel-Onsager equation, ion-solvent interaction, electrochemical polarization, EMF of polarization, decomposition voltage, over-voltage, Butler-Volmer equation, relation between rate of electrochemical reaction and over voltage, principle and applications of cyclic voltammetry.
Reaction dynamics	Kinetics of fast reaction, stopped-flow and relaxation methods for rate measurement, flash photolysis, temperature-Jump method, kinetics of autocatalysis, oscillatory reactions and redox reactions, transition state theory, thermodynamic formulation of reaction rates, potential energy surface and contour reaction path, saddle point, activation energy, Statistical formulation of transition state theory, derivation of expression for specific reaction rate, entropy of activation, pre-exponential factor, single sphere activated complex model, Influence of ionic strength and solvation on reaction rate. Diffusion controlled reactions (full and partial microscopic diffusion controlled), substituent effect and Hammett equation, electron transfer reaction and Marcus theory, reaction in molecular beams, features of potential-energy surfaces, state-to-state kinetics, enhancement of reaction and effect of vibrational and rotational energy, study of transition state species. Spectroscopic observation of chemical reaction dynamics.

Practical (3 h)	Determination of rate constant, influence of ionic strength on reaction rate, determination of thermodynamic and kinetic properties of various chemical systems from spectroscopic observables (peak frequency, amplitude and full-width-at-half-maxima)
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CHY526: Chemistry of Natural Products (L : T : P = 3 : 0 : 0) (Elective Course)

Mother Nature has created plethora of compounds utilizing her biosynthetic tools. These compounds can serve as defense compound against herbivores and pathogens as flower pigments that attract pollinators or as hormones or signal molecules. In addition to these physiological properties, chemistry of natural products has been exploited extensively in the pharmaceutical, agrochemical and fragrance industry. Still 36% of newly emerging drugs are either directly coming natural products or natural product based. Unique structural features of natural products are still a source of inspiration to the synthetic community for new methodology development. In this course, various aspects of the chemistry of natural products will be discussed starting from isolation, characterization, various synthetic approaches to biological activity study. First part of this course will be dedicated to discuss the chemistry of carbohydrate, nucleic acids, lipids, amino acids, proteins and peptides. In the next part, chemistry of alkaloids will be discussed in details. Chemistry of terpenes and steroids will be presented in the last part of the course. Special emphasis will be given to discuss about the biogenesis of alkaloids and terpenoids.

Course content

Introduction of natural product chemistry and classification	Introduction about chemistry of natural products and their application in modern human Society. Classification of various natural products, Biogenesis of primary and secondary metabolites
Chemistry of carbohydrates	Classification, structure and configuration and conformation. Chemistry of monosaccharides and common disaccharides Chemistry of polysaccharides and modern application.
Chemistry of nucleic acids	Structure and functions of nucleosides and nucleotides. Primary and secondary structure of nucleic acids and functions. Chemistry of purine and pyrimidine-based drug molecules (e.g. Zorivax, Retrovir etc.)
Chemistry of lipids	Structure and classification of lipids.

	Chemistry of phospholipids and glycolipids. Recent application of the chemistry of lipids.
Chemistry of amino acids, protein and peptides	Structure, properties and unique features of amino acids. Characteristics, structural and functional Classification of Proteins. Chemistry peptides and peptide-based drug molecules.
Chemistry of Alkaloids and classification	Definition, structure and classification of alkaloids. Proposed biosynthesis of alkaloids. Alkaloids and plants chemical defence
Chemistry of terpenoids indole alkaloids and benzoisoquinoline alkaloids	Chemistry of terpenoids indole alkaloids Chemistry of terpenoids indole alkaloids: continued Chemistry of benzoisoquinoline alkaloids
Application of the chemistry alkaloids in modern medicine	Chemistry and biology of quinine Chemistry and biology of vinblastine Chemistry and biology of vincristine.
Chemistry of steroids: Introduction and classification	Definition, structure and classification of steroids. Characterization of steroids using various spectroscopic techniques. Proposed biosynthesis of steroids.
Chemistry of progesterone, estrone and hydrocortisone	Synthesis of progesterone Synthesis of estrone Synthesis of hydrocortisone
Chemistry of prostaglandins & leukotrienes	Synthesis of prostaglandins. Synthesis of prostaglandins. Synthesis of leukotrienes.
Chemistry of terpenoids: Introduction classification and biosynthesis	Definition, structure and classification of terpenoids. Characterization of terpenoids using various spectroscopic techniques. Proposed biosynthesis of terpenoids
Synthetic strategies of terpene	Synthesis of longifolene Synthesis of jatrofolones Synthesis of cembrene
Application of the Chemistry terpenoids in Modern Medicine	Story of Taxol Application of the chemistry of terpenoids in fragrance synthesis.

and Fragrance	Application of the chemistry of terpenoids in fragrance synthesis.
Problem session for final examination.	Problem session for final examination.

CHY527: Organic Reaction Mechanisms -I (L : T : P = 2 : 1 : 1) (Major Course)

Various mechanistic aspects of organic reactions in the advanced level are designed for the in-class discussion. In the first part of the course, principle and theory related to reactivity, kinetics and mechanism will be demonstrated. Different experimental techniques related to thermodynamics and kinetics will be presented. Furthermore, all newly developed parameters in the field of physical organic chemistry will also be discussed. In the second part of the course, advance stereochemistry and their correlation to mechanism will be discussed in detail. This section will be focused on molecular symmetry and chirality, dynamic stereochemistry, chirality in molecule devoid of chiral centres and molecular recognition. Different types of radical reaction mechanism will be covered in the last part of this course.

Course content

Energy surface, Concepts and Transition State Theory	Energy surface, reaction coordinate and rate constants, Transition State Theory (TST) and its application in studying reaction mechanism, tutorial on energy surface, related concepts and TST.
Postulates and principles of kinetic analysis	Hammond postulate and the Curtin-Hammet principle; Microscopic reversibility & Kinetic vs Thermodynamic control, tutorial on postulates and principles related to kinetic analysis.
Experiments related to thermodynamic and kinetics	Kinetic analysis of organic reaction mechanism and methods for following kinetics, kinetic isotope effects, solvents effects, heavy atom isotope effects and tunneling and tutorial on experiments related to thermodynamic and kinetics.
Linear free energy relationships	Taft parameters, Swain-Scott parameters, Edward and Richte correlation and Winstein plots and Mayer's parameters for the determination of electrophilicity and nucleophilicity, Tutorial on other linear free energy relationships
Thermochemistry of	Stability versus persistence & chemistry of carbanions, chemistry of

reactive intermediates	classical and non-classical carbocations, tutorial on thermochemistry of reactive intermediates.
Relation between structure and energetics-basic conformational analysis	Torsional potential surfaces, gauche interaction, allylic strain, transannular effect and Bredt's rule and conformations of substituted alkenes, Electronic effect: interaction involving π systems, conjugation, aromaticity, orbital effect and effect of multiple heteroatoms, tutorial on conformational analysis.
Molecular symmetry and chirality	Symmetry operations and symmetry elements, point group classifications and symmetry numbers, tutorial on molecular symmetry and chirality
Dynamic stereochemistry: Stereoselective reactions	Stereoselectivity: Classification, terminology, and principle, stereo-selection in cyclic and acyclic systems, tutorial on dynamic stereochemistry.
Chirality in molecule devoid of chiral centers	Stereochemistry of allenes, spiranes, propellers and gears, Stereochemistry of helicenes and molecules with plane of chirality, tutorial on chirality in molecule devoid of chiral centers.
Molecular recognition: Chemical and stereochemical aspects	Chemistry of synthetic molecular receptors and macrocyclic polyethers, enantioselective molecular recognition and its application in catalysis, tutorial on molecular recognition.
General and characterization of free radicals and radical intermediates.	Historical background, long-lived free radicals and detection of free radicals, structure, stereochemical properties and substitution effects, tutorial on general features of free radicals, kinetics characterization of chain reactions, determination of reaction rate and structure-reactivity relationships, tutorial on reaction mechanism of radical reaction.
Various types of radical reactions	Free radical substitution and addition reaction, $S_{RN}1$ substitution reaction of alkyl nitro compound, aryl and alkyl halide compounds, tutorial on radical reactions.
Other types of free radical reactions	Halogen, sulfur, and selenium group-transfer reactions, intramolecular hydrogen atom transfer reactions and rearrangement reactions of free radicals, tutorial on radical reactions
Diastereoselective	Diastereoselective atom transfer and allylation reactions, diastereoselective

radical reactions	radical azidation reactions, tutorial on diastereoselective radical reactions.
Enantioselective radical reactions	Enantioselective radical oxygenation reaction, memory of chirality in H-atom transfer reactions, tutorial on enantioselective radical reactions.
Practical (3 h)	<ul style="list-style-type: none"> • Grignard reaction: Synthesis of triphenylmethanol • Wittig olefination reaction • Friedel-Crafts acylation reaction • Jones oxidation reaction • Synthesis of ibuprofen • Synthesis of carbazoles from naphthols and aryl hydrazine • Synthesis of 1-chloro-3,4-dihydro-2-naphthalenecarboxaldehyde from alpha-tetralone

CHY542: Supramolecular Chemistry (L : T : P = 3 : 0 : 0) (Elective Course)

This course will help to understand the basic concept of supramolecular chemistry and their quantification in molecular recognition processes. This course will cover the area of non-covalent interactions using various examples. This course will also deal with the biological supramolecular systems: Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self- assembly. Supramolecular reactivity Biomimetic systems and Artificial receptors:

Course Content

Basic concept	Principles, History, Molecular recognition
Hydrogen Bonds:	Definition, Structure and Stability, strength, Secondary Electrostatic Interactions in Hydrogen Bonding Arrays
Non-covalent interactions	Ion pairing, Ion-Dipole Interactions, Dipole-Dipole interactions, Dipole-Induced Dipole and Ion-Induced Dipole interactions, van der Waals or Dispersion Interactions, Hydrogen bonding, Halogen bonding, Cation- interactions, Anion-pi interactions, pi - pi interactions, Closed shell interactions,
Aromatic-Aromatic Interactions	Benzene Crystals, Edge-to-face vs. pi-pi Stacking Interactions, N-H- pi interactions, Sulfur-aromatic interactions, Benzene-Hexafluorobenzene pi-stacking.

Biological supramolecular systems	Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly.
Supramolecular reactivity Biomimetic systems and Artificial receptors:	(a) Cation Binding Hosts - Podand, Crown Ether, Cryptand, Spherand; Nomenclature, Selectivity and Solution Behavior; Alkalides, Electrides, Calixarenes and Siderophores. (b) Anion binding hosts - Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods. (c) Ion Pair Receptors - Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction. (d) Hosts for Neutral Receptors -Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins, cucurbituril.
Transport processes	Dynamic Combinatorial chemistry
Chirality	Supramolecular chirality and chirality imprinting
Solid-State Chemistry	Metal Organic Frameworks (MOFs), Covalent Organic Frameworks, Polymorphism, Solvates, Co-Crystals, Salts, Amorphous Materials
Stimuli responsive solids	Topochemical [2+2] cycloadditions in cinnamic acids under light, Topochemical photopolymerization in crystals
Supramolecular Chemistry in Biology	Membranes, Macrocyclic systems, Photosynthesis, Oxygen transport, Biological mimics, Enzymes, Metallobiosites, Heme analogues.

CHY544: Nanotechnology and Nanomaterials (L : T : P = 3 : 0 : 0) (Elective Course)

The next few years will see dramatic advances in atomic-scale technology. Molecular machines, nanocircuits, and the like will transform all aspects of modern life - medicine, energy, computing, electronics and defense are all areas that will be radically reshaped by nanotechnology. These

technologies all involve the manipulation of structures at the atomic level - what used to be the stuff of fantasy is now reality. The economics impact of these developments has been estimated to be in the trillions of dollars. But, as with all new technologies, ethical and legal challenges will arise in their implementation and further development. This course will examine the science of nanotechnology and place it in the larger social context of how this technology may be, and already is, applied. Underlying physical science principles will be covered in lecture sessions and students will read articles from current news sources and the scientific literature. There will be presentations on scientific literature on topics of student interests, to examine the science and applications of a well-defined aspect of nanotechnology of their choosing. Lecture material will focus on the principles behind utility of designed nanostructures for many applications.

Course Content:

- Introduction
- Bulk Vs. Nano
- Different types of nanomaterials – 0D, 1D, and 2D
- Quantum confinement effect
- Surface area to volume ratio
- Effect on Properties: Material (electrical, magnetic, mechanical, optical, etc.) and structural properties
- Carbon nano-architectures: Fullerene, SWNT, MWNT, Graphene, nanodiamonds, etc.
- Nanostructures of silicon and other materials such as germanene, phosphorene, MoS₂, borophene, and some properties
- Q-Dots, nanoparticles of metals and semiconductors, self-assembly, molecular electronics, nanowires
- Bonding parameters
- Methods of preparation
- Nanomaterial's synthesis: Top down and Bottom up approaches, Physical and chemical methods, Applications (Nano-machines, solar cells, coatings, MEMS, nano-medicine, sensors, magnetic storage devices, miscellaneous)
- Characterization Techniques and Instruments (brief overview): Microscopy SEM, TEM, AFM, X-Ray diffraction, UV-vis, Photoluminescence, Raman, FTIR, ESR, XPS, BET, DLS, Zeta potential etc.

CHY545: Fundamentals of Crystallography (L : T : P = 2 : 0 : 1) (Elective Course)

Crystallography in combination with X-ray or neutron diffraction yields a wealth of three-dimensional structural information unobtainable through other methods. The course has been designed to give an overview of crystallography, in general. This basic course will cover the topics such as symmetry in crystallography, crystals systems, Bravais lattices, crystal symmetry, crystallographic point groups and space groups, Miller indices, theory of X-ray diffraction, data collection, data reduction, structure factors and Fourier syntheses, electron density, phase problem, direct methods, Patterson method, crystal structure refinement etc. The course will also highlight the application of single crystal and powder X-ray diffraction techniques and will include hands on training on crystal growth, mounting, structure solution, refinement and analysis. Further, training on the use of database for structural search will also be provided.

Course Content:

Introduction	Introduction on Crystallography and discussion on course structure
Theory of X-ray diffraction	What is X-ray, generation and classification of X-ray, X-ray sources, diffraction of X-rays, Bragg's law, the reciprocal lattice, reciprocal relationship, Bragg's law in reciprocal space, Ewald's sphere, Laue method.
Crystallographic Symmetry	Concept of symmetry and lattices, notations of symmetry elements, 32-point groups and their notations, stereographic projections, Laue symmetry; glide planes, screw axes and their notations, space groups, equivalent points, space group symmetry diagrams etc. Miller Indices, crystallographic planes and directions, close pack structures, Miller-Bravais indices for hexagonal systems.
Data reduction	L-P corrections, structure factor, scaling, interpretation of intensity data, temperature factor, symmetry from intensity statistics, structure factor and Fourier synthesis, Friedel's law; exponential, vector and general forms of structure factor, determination of systematic absences for various symmetry or lattice centering, FFT, Anomalous scattering.
Phase Problem	Definition, Direct Methods, Phase determination in practice, Patterson Methods, Harker line and planes (section), Patterson Symmetry, completion of structure solution, ΔF synthesis.

Refinement of Crystal Structures	Refinement by Fourier synthesis, refinement by ΔF synthesis, Refinement by least squares method, weighting functions, Goodness-Of-Fit (GOF) parameter, treatment of non-hydrogen atoms, and treatment of hydrogen atoms.
Neutron Diffraction	Basics of neutron and synchrotron diffraction and their applications.
Practical (2 h)	Crystal growth, selection, mounting and indexing of crystals, data collection, data reduction, space group determination, structure solution and refinement, introduction to crystallographic packages (e.g. APEX, SHELXTL, ORTEP etc.), IUCr validation of the data, use of both Cambridge Structural Database (CSD) for structural search and International Tables for Crystallography.

CHY547: Chemistry of F-block Elements (L : T : P = 3 : 0 : 0) (Major Course)

In this course, we will discuss the chemistry of F-block elements. Topics in the course includes isolation and purification of lanthanide and actinides elements from natural source, their fundamental descriptive electronic structures, physicochemical, magnetic and photophysical properties, geological sourcing, separations chemistry, supply problems, recycling and sustainability. The course will also focus on aspects related to ligand design for various applications including catalysis, sensing, magnetic resonance and multi-modal imaging agents, and chemistry related to nuclear fuel cycles.

Course content

Introduction	"f" orbitals, oxidation states, atom and ion sizes, lanthanoid contraction, isolation and purification of uranium from natural source, separation using cation exchange resin.
Coordination complex	Coordination complexes of f-block elements, aqueous and redox chemistry, organometallic compounds of uranium, transuranium and transactinium elements.
Spectroscopic and magnetic properties	"f-f" spectra of lanthanides and actinides, luminescence property, bonding parameters and structural evidences from electronic spectra, magnetic behavior of lanthanides and actinides.
Uranium chemistry	Aqueous, redox and complex chemistry of uranium in different oxidation states, simple and complex uranium compounds-their preparation, properties, and reactions, nuclear reactors and atomic energy, nuclear fuel

	reprocessing, Indian scenario.
Applications	Why the global economy treats rare earth metals as 'critical' materials? MRI contrast reagents, sensing, catalysis, smoke detection.

CHY548: Frontiers in Inorganic Chemistry (L : T : P = 3 : 0 : 1) (Major Course)

In this course, the advances in inorganic chemistry will be taught, including learning the concept of physical inorganic chemistry using molecular orbital approach, spectroscopy and reaction kinetics to provide deep understanding in various topics of inorganic chemistry. A special emphasis on chemistry of rings, cluster and cages will be provided. Finally, recent progress on photochemistry and photochemical processes will be discussed.

Course Content

d-d transition	Metal-centered electronic spectra of transition metal complexes: microstates, determination of ground and all excited state terms of d^n ions, splitting of d^n terms in octahedral and tetrahedral fields, qualitative idea of Tanabe-Sugano diagrams, charge transfer spectra according to MO theory.
Magnetochemistry	Magnetic properties of coordination compounds: Spin and orbital moment, spin-orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable-temperature magnetic moments.
Wade's rules	Wade's rules, Carboranes, Metalloboranes. Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, capping rules.
Ring, cluster and cages	Inorganic rings, cages and clusters: Carbide, nitride, chalcogenide and halide containing clusters. Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis. Iso- and heteropolyoxometalates with respect of V, Mo and W: Syntheses, reactions, structures, uses. Metal-metal bonding (M.O. concept), metal-metal bonded dinuclear d-metal complexes-typical examples. Bonding in dirhenium complexes. Syntheses, properties, reactions, structures and bonding as applicable in respect of molybdenum blues, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red, Crutz-Taube complex, Vaska's complex.
Inorganic photochemistry	Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems,

	intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing.
Photochemical processes	Photosubstitution and photoelectron transfer reactions in Co, Cr, and Rh complexes.
Practical (3 h)	<ol style="list-style-type: none"> 1. Qualitative detection: Qualitative detection of cations and anions including lanthanides and actinides. 2. Experiments on quantitative estimation: Analysis of selected ores, minerals and alloys by volumetric, complexometric, gravimetric and other instrumental methods (spectrophotometer etc.) after separation of the components by solvent extraction or chromatographic techniques 3. Synthesis and characterization of inorganic and coordination compounds: Selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands 4. Stability constant measurement: Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric methods

CHY552: Polymer Chemistry and its scope (L : T : P = 3 : 0 : 0) (Elective Course)

How do changing demands in society lead to polymer invention? How are monomers bonded in nature to form our body's building blocks? How do scientists mimic nature in labs? How does the several-fold change in molecular weight from monomer to polymer result in different sets of properties? Most of the polymeric materials around us are synthesized in different ways, depending upon end usage. This course will help to understand the need and importance of polymers in today's world. Interesting chemical aspects of synthesis of polymeric architectures from small molecules will be explored.

Course Content

Introduction	Nomenclature, Classification, Molecular weight, Physical state, Applications
Step Growth Polymerization	Polyamide, Polyesters, Polycarbonates, Phenolic polymers, Epoxy resins, Polyethers, Polyurea, Polyurethanes, Carothers's equation, End group analysis, functional group determination

Chain Growth Polymerization	Free Radical polymerization: Initiators, Inhibitors and retarders, Mechanism, Kinetics and Thermodynamics, Polymerization processes (Bulk, Solution, Suspension, Emulsion), Copolymers
Ionic polymerization	Cationic and Anionic Polymerization: Mechanism, Ring Opening Polymerization (ROP) Controlled/Living polymerizations: ATRP (Atom Transfer Radical Polymerization), RAFT (Reversible Addition Fragmentation Chain Transfer), GTP (Group Transfer Polymerization), Ziegler Natta Polymerization, Metathesis
Specialty Polymers	Conducting Polymers, Liquid Crystal Polymers, Organometallic Polymers, Green Polymers and their applications
Polymer Characterization (Molecular weight determination)	Number average molar mass, End group assay, Colligative Properties of Solutions, Osmometry, Light scattering (Dynamic Light Scattering), Viscometry, Gel Permeation Chromatography, MALDI (Matrix Assisted Laser Desorption/Ionization)

CHY553: Coordination and Bio-inorganic Chemistry (L : T : P = 3 : 0 : 0) (Elective Course)

Metals ions play important role in many biological processes. Understanding of the biological functions of metal ions lies at the heart of bio-inorganic chemistry. This course will focus on the basic concept of coordination chemistry and their quantification in biological processes; for example: dioxygen binding, structure and function of hemoglobin and myoglobin, photosynthesis, iron-sulfur cluster proteins, blue copper proteins, carbonic anhydrase, aldehyde oxidase, Vitamin B12, nitrogen fixation, iron storage and transport proteins, etc.

Course Content

Topics	Learning Objectives
Introduction	Meaning of coordination chemistry and use of metal coordination in biological processes
Structure and bonding	Valence bond theory, Crystal field theory, Molecular orbital theory, MO diagram of CO, O ₂ , CO ₂ , N ₂
Spectra and bonding	Coordination number, bonding of organic ligands to transition metals, isomerism, chelate effect, π -bonding, electronic spectra including MLCT, LLCT, LMCT and magnetic properties of complexes.

Recent development and use of coordination compounds	Metal coordinated cage compounds and their applications
Term paper Presentation	Term paper submission and presentation will be based on the specified subject chosen by the student. Different topic will be assigned for each student (or group).
Metals in Biology	General introduction to importance of metals in biology. Metalloenzymes and metal containing drugs
Metalloporphyrin	Dioxygen binding, Structure and function of hemoglobin and myoglobin
Importance of Iron in biology	Photosynthesis, Iron-sulfur cluster proteins, Transport iron proteins
Importance of Copper in biology	Blue copper proteins, plastocyanin, Stellacyanin, Azurin.
Other metalloproteins	Carboxypeptidase, carbonic anhydrase, aldehyde oxidase, Xanthine oxidase, Vitamin B12, Metallothioneins.
Nitrogen fixation	Mechanism of nitrogen fixation, in vitro and in vivo nitrogen fixation.
Metals in medicine	Antibiotics and related compounds, anticancer drug cisplatin and related metal complexes.
Recent advances	Group of students will be assigned some literature survey on recent important papers related to the course so that they can have some idea on the recent advances on the importance of metals in bioinorganic chemistry and drug discovery.

CHY 554: Green Chemistry and Sustainability (L : T : P = 3 : 0 : 0) (Elective Course)

Since a decade, scientific community especially chemistry has been mobilized to develop new chemistries that are less hazardous to human health and the environment. Several steps were taken to protect both the nature and maintain ecological balance. But still such an effort is in nascent stage. Are we really protecting earth? Are we utilizing nature's sources wisely? What are the hazards associated with one wrong step and with several such steps? We are surrounded by chemistry since we wake up in morning until, we sleep in night such as toothpaste, soap, cloth, perfume, medicine, plastic furniture, shoes etc. For those of us who have been given the capacity to understand chemistry and practice it as our day-to-day life, it is and should be expected that we should use it in a sustainable manner. With knowledge comes the burden of responsibility. We should not enjoy this

luxury with ignorance and cannot ignore the effects of the science in which we are engaged. A joint effort to work hard and put brain waves together is desired to develop and align new and old chemistries that are more benign, and safer to mother earth!

Course Content

Green chemistry	Lessons from past for a better future: Need, Limitations and Opportunities Principles of Green Chemistry and their illustrations with examples: Scales of measurement such as Atom efficiency, E factors etc., homo vs. heterocatalysis, reaction efficiency, toxicity reduction etc.
Green reactions	Green alternatives of starting materials, non-risky reagents, benign solvents (Aqueous medium, Ionic liquids, Supercritical fluids, Solvent free reactions), and reaction conditions (Nonconventional energy sources: Microwave assisted reaction, Ultrasound assisted reactions, Photochemical reactions), catalysis (heterogeneous catalysis, biocatalysis, phase-transfer catalysis), Replacement of Non-Green reactions with Green reactions (Real/Award cases)
Oxidative catalyst synthesis principle using first row transition metal	C-H activation, epoxidation, O-H activation, C-C bond coupling
C-H activation	Organometallic C-H activation vs. Metal-oxo catalyzed C-H activation. Selectivity in C-H activation.
Water Oxidation	Green energy source, water splitting, water oxidation in acidic and alkaline condition, photochemical water oxidation, electrochemical water oxidation, photo-electrochemical water oxidation
CO ₂ fixation	Overview of pathways, Oxygenic photosynthesis, Bacteria and cyanobacteria, Other autotrophic pathways
Decontamination of pesticides in soils	Pesticide, insecticide and herbicide decontamination

CHY556: Inorganic Reaction Mechanism (L : T : P = 3 : 0 : 0) (Elective Course)

The aim of this course is to teach the basic mechanisms of inorganic reaction types, such as electron transfer reactions, ligand substitution reactions and the reactions of organometallic compounds.

Inorganic reaction mechanisms available in the literature will be used to solve chemical problems. The interpretation of modern concepts of inorganic reaction mechanisms helps to consolidate and integrate the knowledge amongst class. Journal article presentations will be held in class weekly.

Course content

Introduction	General discussion about reaction kinetics, how to derive rate law and the ambiguity of mechanistic interpretations of rate laws
Substitution reaction	Four broad classes of mechanism of substitution – ‘D’, ‘A’, ‘Ia’ and ‘Id’. Mechanism of isomerization reaction – linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, inorganic substitution reaction for octahedral geometry vs. square planar geometry, trans effect vs. trans directed effect.
Electron transfer reaction	Outer sphere ET vs. Inner sphere ET vs. Proton coupled ET (PCET).
Reactions of coordinated ligands	Insertion, Oxidative addition, Reductive elimination.
Catalysis without precious metal	Homogeneous catalysis, C-H functionalization vs. C-H activation, organometallic C-H activation vs. biological C-H activation, photocatalysis.

CHY557: Intelligent Materials for Nanomedicine (L : T : P = 3 : 0 : 0) (Elective Course)

Recent advances in field of medicine have resulted in designing and development of large number of novel synthetic architectures for target drug delivery in order to revolutionize the treatment and prevention of disease. Advanced drug delivery and targeting can offer significant advantages to conventional drugs, such as increased efficiency, safety for drug delivery, convenience. However, such potential is severely compromised by significant obstacles to delivery of these drugs in vivo. These obstacles are often so great that effective drug delivery and targeting is now recognized as the key to effective development of many therapeutics including theranostics. This course will provide a comprehensive introduction to the various carriers for drug delivery, principles of advanced drug delivery and targeting, their current applications and potential future developments.

Course Content:

Introduction	Introduction to intelligent materials and structures
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Principles of Drug delivery systems (DDSs)	What are the principles of DDSs? Why drug delivery is important for better efficacy? How to deliver the drugs using carriers at targeted site and control the drug release rate, drug absorption and overcome the limitations of drug resistance and enhances the therapeutic effects. Drug concentration at the targeting site should persist in the therapeutic window.
Nanocarriers for Drug Delivery	Basic properties, classifications of the nano-carrier: Organic, polymeric and inorganic
Design of Organic and Polymer-Based DDSs:	<p>Commercial sources, synthetic methods, capsules/vesicles, their methods of preparations such as emulsification, Layer-by-Layer assembly, coacervation, internal phase separation, flow focusing devices.</p> <ul style="list-style-type: none"> I) Polymer-based Amphiphilic Nanocarriers II) Micelle and Vesicle Nanocarriers from Polymer-Based Amphiphiles, <ul style="list-style-type: none"> a. Poly(lactic Acid) (PLA), (PLGA) Copolymers, b. Chitosan c. Temperature-Sensitive Polymeric Nanocarriers (Thermosensitive Poly(<i>N</i>-isopropylacrylamide) (PNIPAm), thermo-responsive (Pluronic) d. Polymeric Nanogels III) Liposome nanocarriers IV) Dendrimers
Approaches for shell wall disassembly/ release	<p>Chemical changes (switching, shell wall disintegration), cross-link removal; Bulk changes (pressure-induced rupture, shell wall melting, changes in porosity, thermomechanical degradation of the shell wall).</p> <p>Physical and chemical triggering phenomena: Chemical triggers, pH-responsive materials, biologically induced reactions, thermally induced release/ temperature responsive, electrical, magnetically initiated triggering.</p>
Materials capable of molecular recognition	Cellular targeting, recognition reagents
Nanotechnology in medicine: Nanoparticles in drug delivery:	<p>Novel delivery modalities: Active targeting and passive targeting DDSs, advantages and disadvantages</p> <p>Design of inorganic based DDSs (Inorganic nanoparticles):</p>

Nanomedicine Formulations:	I) Carbon Nanotubes, II) Gold Nanoparticles (Au NPs), III) Quantum Dots (QDs), IV) Superparamagnetic Iron-Oxide Nanoparticles (SPIONs), V) Mesoporous Silica Nanoparticles, VI) Organic/Inorganic Hybrid Nanocarriers Clinical Development and Approved Materials
Toxicity of metallic nanoparticles:	Is it safe for metal-based nanoparticles for medicinal applications?
Applications of nanomaterials to biology or medicine and future Perspectives	Cancer therapy (Thermal therapy) Diagnostic testing (Optical, magnetic, SERS) Future Perspectives

CHY558: Organometallic Chemistry (L : T : P = 3 : 0 : 0) (Elective Course)

The aim of the course is to describe how modern organometallic chemistry is bridging classical organic chemistry and traditional inorganic chemistry. Emphasis will be given on structure and bonding, reactivity and applications of organometallic complexes in organic synthesis and industrial catalysis.

Course Content

Main group organometallics	Classification, syntheses, reactions, structure and bonding and applications of typical examples; Use of nontransition metal aluminum, indium, germanium, tin, lead <i>etc.</i> , Chemistry of organosilane: hydrosilylation; Multiple bonds between silicon atoms; Silicon in =1 and 0 oxidation state; Frustrated Lewis pairs (FLPs) as catalyst in organometallics.
Fluxionality	Stereochemical non-rigidity and fluxional behavior of organometallic compounds with typical examples.
Reactions of organometallic	Substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

complexes	Innocent ligands, non-innocent ligands, redox active ligands and phosphines and N-heterocyclic carbenes.
Asymmetric synthesis	Asymmetric hydrogenation and hydroformylation; Detailed reaction mechanism; Chiral catalyst deactivation pathway
Olefin metathesis	Grubb's catalyst; Idea behind the development of 1st generation to 2nd generation Grubb's catalyst; Mechanistic explanation.
Application	Application of organotransition metals in organic synthesis-preparative, structural and mechanistic aspects; Green-Davies-Mingos rule; Catalytic nucleophilic addition and substitution reaction; Pauson-Khand reactions; Volhardt co-trimerisation; functional organometallic compounds. Synthetic applications of (a) transition metal complexes containing metal-carbon sigma-bonds (b) reactions of transition metal carbonyl complexes (c) transition metal carbene complexes (Fisher carbene and Schrock carbenes and their applications in the synthesis of organic molecules) (d) transition metal alkene, diene, and dienyl complexes (e) synthetic applications of transition metal alkyne complexes

CHY600: Research Methodology (L : T : P = 2 : 0 : 0) (Major Course)

In this course, students will learn about various scientific methods that we commonly use in research. However, the primary focus will be to teach how to become a good researcher/ scientist. The course will comprise various sections covering the dos and don'ts of science, integrity and honesty, reading-writing-presentation skill as well as scientific techniques. Classes will be through a combination of lectures, reading articles and presentations. Students are expected to do literature research, read articles, discuss and present in the class. Relevant articles to be supplied by the instructor(s).

Introduction	Overview Lecture
Ethics, Academic dishonesty, plagiarism, Lab safety	Overview lecture on publication ethics, especially Data fabrication and falsification, Plagiarism, Improper author contribution or attribution. In addition, the lab safety is key important. What are the safety rules and why these are important for safe working environment?
Plan/design of experiments/Theory and	How students can plan for new research in the beginning of research career including M.Sc. research and PhD. Identifying the research

Maintaining notebook	problem and how to design the experiments to address these issues. After planning of the experiments, how to conduct the experiments in wet lab or theoretical analysis. The progress of research needs to record systematically.
Literature search from available search engine and Writing research proposal, manuscript, project/work report etc.	Purpose of literature survey (periodically) and gaining in depth knowledges of specific research area in which students are interested. Most useful search engine will be demonstrated. How to identify the research gap and highlight the key findings of research in your manuscript. Especially how to write your data especially which tense is appropriate for methodology and discussion of your manuscript.
Slides preparation and presenting research work effectively (communication skill development)	Preparation of good power point presentation (PPT) is an art. Here tips for preparing effective PPT will be demonstrated/discussed. The layout of presentation, use of contrasting colors for text and background/ the front size/ animation and so on will be discussed.
Reading, understanding and presenting research articles	Students need to get to the habit of reading research articles. May need multiple reading to understand the results and get ideas for their own research works. Students will be provided with the recent research articles, based on which presentation to be delivered with focus on aim of the research and their findings and student's learning outcomes.
Writing skill development	Students need to understand and analyze some given schematic diagrams/ graphical abstracts/ figures and results (experimental or theoretical) and discuss the same in the form of manuscript/report.
Data handling, data analysis and statistical methods	How to handle (large) data set efficiently using computational tools? What is error analysis? What are the different error estimation methods? Which tool could be appropriate for a given data type? Students need to demonstrate the utility of such tools for a given data set.

This course will deal with Data handling and Data Analysis, elements of Qualitative and Quantitative Logic, including Hypothesis testing, Weight of Evidence, and Domain of Applicability estimation. Other topics to be discussed include Bayes rule, distribution functions, statistical validation, assessment metrics, and reproducibility in science.

CHY609: Strategies for problem solving (L : T : P = 2 : 0 : 0) (Elective Course)

In this course, problem solving strategy will be taught through lecture, tutorial and home assignments. The courses will provide a journey of various subjects learnt and utilize them on how to approach and answer several question problems. Especially several questions and answers on physical chemistry syllabus such as basic principles of quantum mechanics, atomic structure chemical bonding, molecular spectroscopy, applications of group theory, thermodynamics, electrochemistry, chemical kinetics, polymer chemistry and colloids and surfaces will be discussed. Similarly, inorganic syllabus such as chemical periodicity, VSEPR theory, coordination compounds, acids and bases, main group elements and their compounds, transition elements and CFT, organometallic compounds, metal cluster Bioinorganic chemistry, analytical chemistry and nuclear Chemistry will be taught. In addition, organic chemistry such as IUPAC nomenclature, aromaticity, principles of stereochemistry, organic reactive mechanisms and intermediates, organic reagents, and synthesis including asymmetric synthesis, named reactions, pericyclic reactions, and structure determination of unknown organic compounds using spectroscopy and spectrometry-techniques. It will also cover chemistry in nanoscience and technology, bioorganic chemistry including carbohydrates, proteins, nucleic acids, catalysis and, supramolecular chemistry.

CHY611: LASER spectroscopy (L : T : P = 3 : 0 : 0)(Elective Course)

The invention and the development of laser revolutionized many branches of science including chemistry. Now a day's laser spectroscopy is often used to measure properties, composition and transformation of chemical compound in real time, thus it becomes an essential tool in chemistry. This course will provide a fundamental understanding of spectroscopic techniques that use lasers and the essential theories. Theoretical background and physical properties of laser, generation, properties and measurement of ultrashort laser pulses, non-linear optics and frequency conversion processes will be covered in the course. Instrumentations for a number of modern laser spectroscopic techniques, detection of optical signal and contemporary chemical research in the field including ultrafast dynamics of chemical and biochemical systems will also be discussed.

Course content

Physical properties of laser	Principles of laser action, properties of laser light, interaction between light and matter
Various laser systems	Nd:YAG laser systems, Ti:sapphire laser systems, Semiconductor diode lasers
Ultrashort laser pulse	Electromagnetic field in the optical resonator, generation of ultrashort laser pulses, Q-switching and mode locking, pulse amplification, chirped pulse amplification, measurement of ultrashort pulse
Nonlinear optics	Nonlinear polarization and nonlinear optical phenomena, non-linear crystals, various frequency-mixing processes, frequency doubling and tripling, phase matching
Introduction to several laser spectroscopic techniques	Instrumentation of laser spectroscopy and detection of optical signal, spatial and temporal coherence, coherent superposition of quantum states and the concept of wave packets, selected spectroscopic techniques in laser chemistry, laser-induced fluorescence spectroscopy, laser induced breakdown spectroscopy (LIBS), pump-probe spectroscopy, stimulated Raman and coherent anti-Stokes Raman spectroscopy, two-photon (multi-photon) excitation, photoionization, ionization spectroscopy
Femtosecond laser chemistry	Femtochemistry: chemistry in the fast lane, transition-state spectroscopy, femtosecond optical gating, photon echo spectroscopy, solvation dynamics, ultrafast electron transfer, proton transfer and isomerization reactions, energy selectivity: mode-selective chemistry, lasers in medicine
Laser microscopy	Fluorescence microscopy, confocal microscopy and stimulated emission depletion (STED) microscopy and their application in chemistry and biochemistry

CHY616: Statistical Mechanics (L : T : P = 3 : 0 : 0) (Elective Course)

In this course, ensembles in statistical mechanics, non-interacting and interacting systems, simulations of statistical systems, non-equilibrium statistical mechanics will be covered.

Course content

Thermodynamics and	1.1 Thermodynamic Equilibrium state
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Mechanics	<ul style="list-style-type: none"> 1.2 Laws of thermodynamics 1.3 Axiomatic formulation of thermodynamics 1.4 Thermodynamic potentials 1.5 Stability criteria 1.6 Phase equilibria 1.7 Classical and Quantum Mechanics 1.8 Hamiltonians 1.9 Transport theory 1.10 Boltzmann H-theorem
Ensembles in Statistical Mechanics:	<ul style="list-style-type: none"> 2.1 Ensemble postulate and ergodicity 2.2 Micro-canonical, canonical and grand canonical ensembles 2.3 Quantum and classical partition functions 2.4 Phase space 2.5 Fluctuations
Non-interacting systems	<ul style="list-style-type: none"> 3.1 Factorization of the partition function 3.2 Quantum correlations 3.3 Collective modes 3.4 Occupation numbers 3.5 Collections of fermions, bosons and photons 3.6 Classical ideal gas of spinless particles 3.7 Molecular partition functions 3.8 Ideal paramagnets and superconductivity
Interacting Systems	<ul style="list-style-type: none"> 4.1 Configurational Partition functions 4.2 Pair correlation function 4.3 Virial equation and Meyer cluster diagrams. 4.4 Phase Transitions in Lattice models Lattice gas 4.5 Ising Model, order parameter, Mean Field theory,
Simulations of statistical systems:	<ul style="list-style-type: none"> 5.1 Computer Simulations and Ensemble averages 5.2 Ergodicity and random numbers 5.3 Monte Carlo methods 5.4 Molecular Dynamics at different ensembles
Application	<ul style="list-style-type: none"> 6.1 Linear Response theory 6.2 Fluctuation dissipation theorem 6.3 Time correlation functions 6.4 Applications of transport phenomena

CHY619: Advanced Quantum Chemistry (L : T : P = 3 : 0 : 0) (Major Course)

Quantum chemistry offers a quantitative view of molecules and accurately predict chemical and physical properties of molecules. In this advanced course, discussion on electronic structure calculations including density functional theory in the stationary state, time-dependent quantum mechanics (TDQM) and their applications at the frontier of research in physical chemistry will be co majorly considered. As time evolution of quantum mechanical systems is important in physical chemistry, a significant portion of the course will deal with time-dependent Hamiltonian, time evolution operator, density matrix analysis etc. The course also includes quantum theory of open system, ab-initio molecular dynamics and molecular simulation using QM/MM method.

Course content

Time-Independent Quantum Mechanics	Formalism of Quantum Mechanics Quantum Mechanics of vibration and rotation Born-Oppenheimer approximation
Mean field theories	The Hartree-Fock self-consistent field method Density Functional Theory Modern exchange-correlation functional
Time-Dependent Quantum Mechanics	Time-evolution Operator Solution of Time-Dependent Schrodinger Equation: Schrodinger, Heisenberg and Interaction Pictures Two-level systems Time-Dependent Perturbation Theory: Rabi Oscillation, Fermis Golden Rule
Mixed State and Density Matrix	Density Matrices, Density Operator and Bloch formalism Energy Representation of the Density Operator: Coherences Time-Evolution of Density Matrix: Liouville-Von Neuman Equation Diagrammatic Perturbation Theory
Electron Density Distribution	Quantum Mechanical Treatment of Molecules: Natural Orbitals and NBO Analysis
Quantum Theory of Open Systems	System-bath interaction; Atoms in Molecules
Ab-initio Methods	Born-Oppenheimer Molecular Dynamics QM/MM Formalism

CHY621: Organic Named Reactions II (L : T : P = 3 : 0 : 0) (Elective Course)

Several named reactions and their reaction mechanism focusing on substitution, addition, elimination and rearrangements of C-C, C-N and C-O are addressed in this course. Stereo selective bond formation and their mechanisms with examples are the key highlights here. Here, these types of selective oxidation, reduction, amination, photochemical reactions and rearrangement reactions leads to specific name reactions. Useful, valuable, and important strategy for organic synthesis will definitely be helpful for advanced students and researchers in the field of organic synthesis. Herein, how these name reactions are useful tool for the synthesis of drug, inhibitors like complex molecules are summarized with various examples.

Course Content

Rearrangement Reactions	<ol style="list-style-type: none">I. Aza-Cope RearrangementII. Aza-Claisen RearrangementIII. Amadori RearrangementIV. Bergman cycloaromatizationV. Ciamician-DennstedtVI. Cope Elimination Reaction/ Oxy-Cope RearrangementVII. Fischer-Hepp Rearrangement (Nitrosamine Rearrangement)
Functional group interconversion	<ol style="list-style-type: none">I. Arndt-Eistert SynthesisII. Baeyer-Villiger ReactionIII. Nef ReactionIV. Barton ReactionV. Leuckart reaction
Coupling Reactions C-C and C-N	<ol style="list-style-type: none">I. Baylis-Hillman ReactionII. Buchwald-Hartwig Cross CouplingIII. Glaser couplingIV. Gomberg-Bachmann reactionV. Trost Allylation (Tsuji-Trost Reaction)
Aromatic Substitution/Aromatic ring formation	<ol style="list-style-type: none">I. Bernthsen Acridine SynthesisII. Blanc chloromethylation:III. Bischler-Napieralski ReactionIV. Bucherer Carbazole SynthesisV. Bucherer Reaction

	VI. Pschorr Reaction VII. Vilsmeier-Haack Reaction VIII. Von Richter Rearrangement IX. Hoch-Campbell Aziridine Synthesis X. Chichibabin Reaction
Synthesis of Alkenes and oxidations reactions	I. Chugaev elimination II. Dakin Oxidation III. Dess-Martin Oxidation IV. Elbs Reaction/ Elbs Persulfate Oxidation (Phenol Oxidation) V. Jacobsen Epoxidation VI. Julia Olefination VII. McMurry Coupling Reaction VIII. Milas Hydroxylation of Olefins IX. Pfitzinger Reaction X. Shapiro Reaction XI. Stork Enamine Reaction XII. Swern Oxidation (Moffatt-Swern Oxidation)
Miscellaneous Reaction	I. Henry Reaction (Nitroaldol Reaction) II. Graebe-Ullmann Synthesis III. Pinner Triazine Synthesis IV. Michaelis–Arbuzov reaction V. Simmons-Smith Reaction

CHY627: Organic Reaction Mechanisms – II (L : T : P = 2 : 1 : 0) (Elective Course)

In this course, various modern trends in organic chemistry will be discussed in detail. Mechanistic details of modern photochemical reactions and classification of different types of photochemical reaction will be discussed. The principles underlying various catalytic reactions and their application will be discussed. Additionally, both C-H bond functionalization (aromatic and aliphatic) and C-H activation will be discussed to understand their utility in designing various molecules of biological and pharmaceutical relevance.

Course content

The Jablonski Diagram & bimolecular photophysical process.	Electromagnetic radiation, absorption and radiation less vibrational relaxation. Phosphorescence, fluorescence, internal conversion and intersystem crossing. Tutorial on photophysical process.
Orbital symmetry consideration of photochemical reactions	Orbital symmetry consideration. Photochemistry of alkenes, dienes, polyenes. Tutorial on photochemical reactions.
Photochemical reaction	Photochemistry of carbonyls and aromatic compounds. Cis-trans isomerization via photochemical reactions. Tutorial on photochemical reactions
Photochemical reaction	Photochemistry of aromatic compounds and photochemical rearrangement reactions. Hydrogen abstraction and fragmentation reaction. Tutorial on photochemical reactions.
(Principles of Catalysis and it's application in catalytic reaction design)	Binding the transition state better than the ground state. Thermodynamics and kinetic aspects of catalysis. Tutorial on the general aspects of catalysis.
Various types of catalysis.	Electrophilic and nucleophilic catalysis. acid-base catalysis. Tutorial on the various types of catalysis. Covalent and non-covalent catalysis. phase transfer catalysis. Tutorial on the various types of catalysis.
Enzymatic Catalysis	Michaelis-Menten Kinetics and the meaning of Michaels-Menten Kinetics. Enzyme active site, reaction coordinate diagram and supramolecular interactions. Tutorial on enzyme catalysis.
(Principles of aliphatic C-H bond activations and functionalization) Mechanistic aspects of aliphatic C-H bond activations	Historical perspective of aliphatic C-H bond activations and functionalization. Key concepts of various modes of aliphatic C-H bond activations and functionalization. Tutorial on Mechanistic aspects of aliphatic C-H bond activations.
Review on organometallic reaction mechanism	Various types of oxidative additions and migratory insertions. Mechanistic understanding of transmetallation. Mechanistic understanding of reductive elimination.
Undirected	Functionalization of aliphatic C-H Bonds by Carbene Insertions.

Functionalization of Alkyl C-H Bonds	Alkylative Carbonylation and borylation of Alkanes. Tutorial on Undirected Functionalization of Alkyl C-H Bonds.
Directed Functionalization of Alkyl C-H Bonds	Directed Oxidations, Aminations, and Halogenations of Alkanes. Directed Hydroarylation of Olefins and alkynes. Tutorial on Directed Functionalization of Alkyl C-H Bonds.
Principles of aromatic C-H bond activations and functionalization, Aromatic C-H Bonds	Borylation and silylation of aromatic C-H bonds. Alkylative Carbonylation of Arenes. Tutorial on undirected functionalization of aromatic C-H bonds.
Directed Functionalization of Alkyl C-H Bonds.	Directed Oxidations, Aminations, and Halogenations of Arenes. Intermolecular and intramolecular aromatic C-H bond functionalization by carbene Insertion. Tutorial on directed functionalization of aromatic C-H bond.
Ligand directed functionalization of aromatic C-H bonds.	Ligand directed functionalization of para--aromatic C-H bonds Ligand directed functionalization of meta--aromatic C-H bonds. Tutorial on ligand directed functionalization of aromatic C-H bonds.
Application of aromatic and aliphatic C-H bond activations and functionalization.	Application of aromatic and aliphatic C-H bond activations and functionalization in the synthesis of pharmaceuticals and natural products. Problem session for final examination.

CHY644: Chemistry of Materials (L : T : P = 3 : 0 : 0) (Major Course)

Chemistry of materials is at the forefront of the fundamental and applied research in materials for the advancement of society and high technology development. It interfaces with chemistry, chemical engineering, life science, and materials science and therefore has interdisciplinary character. Currently this subject draws great attention both from theoretical and experimental studies with a focus on the preparation, design, and understanding of materials with unusual, distinguishable and characteristic properties with several relevant useful applications. Studies of crystals in different dimensions, nanomaterials, and polymers of both inorganic and organic materials; fabrication and processing of materials/devices to form self-organized molecular assemblies with novel sets of properties, and design of optimal materials are emerging areas of materials research. Theoretical aspect and

prediction of stable structures guide the experimental outputs and play a distinct role to dictate remarkable properties. For a student of chemistry, it has become imperative to learn many aspects of materials involving design, synthesis, investigation, application of polymeric and molecular precursors to solid-state inorganic materials and the preparation and study of bio-/nano-materials, composites, catalysts, liquid crystals, coatings, thin films and interfaces, to name a few.

Course content

Structure and bonding	Overview of Bravais lattices and crystal systems, primitive lattice vectors, Wigner-Seitz cell, symmetry in crystals, x-ray diffraction, reciprocal lattice, structure factor, defects, different types of bonding in materials.
Electronic, magnetic, vibrational, and optical properties	Free electron model, electrical conductivity and Ohm's law, Bloch's theorem, band theory and band gap, metals, semiconductors, and insulators, intrinsic and extrinsic semiconductors, p-n junctions and transistors. Lattice vibrations - phonon spectrum, lattice heat capacity; thermal expansion; Thermal conductivity. Magnetic materials – Paramagnetism, Langevin diamagnetism, ferro, anti-ferro and ferrimagnetism, magnetic domains and hysteresis, superparamagnetism. Optical properties – reflectance, plasmon frequency, Raman scattering in crystals, optical absorption, photoconduction, photo and electroluminescence, lasers.
Introduction to different materials and relevant properties	Polymers, amorphous and quasicrystalline materials, alloys and compounds, nanomaterials
Materials for energy	Photovoltaic and photo-chemical effects, Exposure to material design for photovoltaic, LED/OLEDs, batteries, supercapacitors, and issues on energy conversions
Organic-inorganic materials	Phosphazene, borazines, TMDs: Synthesis, properties, bulk and nanostructures and important applications.

CHY649: Analytical Chemistry (L : T : P = 3 : 0 : 1) (Major Course)

Basics of measurements and data analysis. Introduction to spectrometric methods and components of optical instruments. Atomic absorption, fluorescence, emission, mass, and X-ray spectrometry (X-ray photoelectron spectroscopy (XPS), X-ray absorption near edge structure (XANES), X-ray absorption spectra (XAS), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction). An introduction and applications to various techniques will be discussed: Molecular absorption (ultraviolet-visible), luminescence, infrared, nuclear magnetic resonance, and mass spectroscopy/spectrometry; electroanalytical methods (potentiometry, coulometry, and voltammetry); chromatographic separation (gas, high-performance liquid, supercritical fluid, and capillary electrophoresis chromatography); thermal methods of analysis; circular dichroism (CD), transmission electron microscopy (TEM), scanning electron microscopy (SEM).

Course content

Measurement and Data Analysis	Classification and Selection of Analytical Methods, Types and Calibration of Instruments, Signals and Noise, Linear and Nonlinear Regression Analysis.
Components of Optical Instruments	General Designs of Optical Instruments, Sources of Radiation, Wavelength Selectors, Sample preparations, Radiation Transducers, Signal Processors and Readouts, Types of Optical Instruments, Principles of Fourier Transform Optical Measurements
Atomic/Molecular Absorption spectroscopy, Fluorescence, Emission spectroscopy, Mass, and X-Ray Spectrometry	Atomic/molecular Absorption Instrumentation, Interferences in Atomic Absorption Spectroscopy, Atomic/molecular Absorption Analytical Techniques, Atomic/molecular Fluorescence Spectroscopy, Emission Spectroscopy Based on plasma, Arc and Spark Sources, Introduction to molecular Mass and X-Ray Spectrometry.
Mass Spectrometry/ ICP mass spectrometry	Molecular Mass Spectra, Ion Sources, Mass Spectrometers, Applications of Molecular Mass Spectrometry, Quantitative Applications of Mass Spectrometry. Applications of Inductively coupled plasma mass spectrometry (ICP-MS). Comparison among different mass analysis techniques. Advantages and disadvantages.
Introduction to Electroanalytical Methods -	Types of Electroanalytical Methods: Conductometry, Electrogravimetry, Coulometry, Voltammetry Instruments for

Potentiometry, Coulometry, and Voltammetry	Measuring Cell Potentials, Direct Potentiometric Measurements, Potentiometric Titrations, Current-Voltage Relationships During an Electrolysis. Coulometry: Potentiostatic Coulometry, Coulometric Titrations (Amperostatic Coulometry), Voltammetry: Cyclic Voltammetry, Polarography, Stripping voltammetry.
Chromatographic separations and techniques	A brief overview on theory followed by practice and instrumentation associated with chromatographic separation techniques will be discussed. The focus is primarily on High Performance Liquid Chromatography (HPLC) and Gas Chromatography (GC), Ion Chromatography (IC), Size-Exclusion Chromatography (SEC), electrophoresis and reverse-phase bio-separations. How the interface with hyphenated techniques involving Mass Spectrometry (MS), such as LC-MS and GC-MS, will be briefly covered. Alternative approaches as a replacement for liquid to supercritical fluid and other greener approaches will be discussed. Examples will be shared and discussed to correlate type of chromatography with separation of compounds (troubleshooting). Issues faced and probable approaches available will be studied with case studies.
Introduction to Thermal Methods of Analysis	Thermogravimetric Methods (TG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC).
Introduction and applications of electron microscopy	Introduction to and applications of transmission electron microscopy (TEM), scanning electron microscopy (SEM). Image J software to analysis the size of the nanoparticles.
Practical (2 h)	<ol style="list-style-type: none"> 1. Analysis of given organic samples by using 1D and 2D NMR (COSY, NOESY) Heteronuclear through-bond correlation methods (HSQC, HMBC) and DEPT. (Data analysis) 2. Absorption and emission spectroscopic analysis of given commercial dyes to understand their nature of ground and excited states (Data analysis) 3. Calibration and HPLC separation of Benzoic acids and 4-Amino acetophenone (practical and data analysis)

	<ol style="list-style-type: none"> 4. Estimation of benzaldehyde and toluene in Gas chromatography (practical and data analysis) 5. Detection of non-UV active compound (glucose/sucrose) using evaporative light scattering detector (ELSD) in Flash chromatography/Prep-HPLC. 6. TGA study for loss of moisture, drying, thermal stability of materials (organic and inorganic) ($\text{CuSO}_4 \cdot x\text{H}_2\text{O}$) (practical and data analysis) 7. Bandgap analysis of Alq3 complex by using UV-vis and Cyclic voltammetry. (practical and data analysis) 8. Study of crystallization (exothermic), melting (endothermic), glass transition of small organic molecule through DSC technique. (practical and data analysis) 9. Structure determination of given unknown organic samples by using NMR, UV-vis, IR, LC-MS techniques (Data analysis).
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CHY352/CHY652: Advanced Biochemistry (L : T : P = 3 : 0 : 0) (Elective Course)

The course is designed to explain the biochemical reactions by the knowledge of chemistry. The transition of the knowledge acquired in chemistry will be nurtured to understand the functions of biomacromolecules such as nucleic acids, proteins, carbohydrates and lipids. In addition, how these biochemical reactions occur by help of the vitamins, enzymes and hormones in different subcellular organelles. We will also learn the chemistry and biochemistry associated with these biomacromolecules with examples. The goal is to learn the importance of the chemistry associated to these biomolecules including carbohydrate metabolism, Protein Sequencing, DNA Sequencing, DNA chemistry, Gene Sequencing, Co-factors, Co-enzymes. Classes will be through a combination of lectures, presentations and assignments.

Course content

Introduction	Biomolecules: Carbohydrates, Proteins, Nucleic Acids, Lipids, Enzymes and Vitamins
Carbohydrates	Structure and Functions; Carbohydrates metabolism; Kreb's Cycle and Glycolysis.

Proteins & Protein Sequencing	Properties, Structure and Functions, Protein Sequencing, Edman degradation, Sanger's reagent and Dansyl chloride Sequence by Mass Spectrometry (MALDI, ESI-MS, Tandem MS)
Nucleic Acids & DNA Sequencing	Introduction of Nucleic acids; DNA Translation, Gene expression, Genetic Code; DNA Sequencing; Sanger dideoxy method; Maxam Gilbert; Bisulfite
DNA chemistry	DNA damage; Methylation and deamination, depurination; Oxidative DNA damage; DNA-DNA crosslinks; DNA-Protein crosslinks; Mutagenesis; Diseases and carcinogenesis
DNA Repair and recombination	Base excision Repair (BER), Mismatch excision Repair (MER), Nucleotide excision Repair (NER),
DNA replication & PCR	PCR, qPCR, RT-qPCR and Reverse Transcriptase-PCR (RT-PCR) techniques.
	Forensics, Relationships, and medical Diagnosis
Lipids	Fatty Acids, Classes of Lipids; Nomenclature of fatty acids; Examples of diff. Lipids; Phospholipids; Steroids
Enzymes	Co-factors, Co-enzymes, Apo-enzyme, Halo enzymes; Factors effecting Enzymes (Con., pH, T); Nomenclature, Mechanism of Enzymes; Biosynthesis of cofactors; NAD ⁺ -NADPH; Biosynthesis of Niacin (Vitamin B3); FAD-FADH-FADH ₂ ; Thiamine pyrophosphate TPP
Hormones and Vitamins	Classifications of Hormones, Examples and Function of Hormones Classifications of Vitamins; Examples and Function of Vitamins

CHY899: Seminar (L : T : P = 1 : 0 : 0) (Major Course)

In this course, skills to present recent literature, more specifically in the area of latest and relevant area of research interest, effectively will be taught using international repute journals. Students will develop skills on how to read, analyze and categorize research publications. Scientifically and that too in their own manner will help them to develop research interests. The presentation given will be judged critically by the faculties. Skills on how to prepare good slides, manage time provided for presentation and improve the presentation skills will be answered. Furthermore, in depth understanding on specific subject through open discussion with students and faculties will allow to develop personality, ability to initiate dialogue and interact confidently.

