SHIV NADAR
INSTITUTION OF EMINENCE DEEMED TO BE
UNIVERSITY
DELHI NCR

Post-Graduate Catalogue

DEPARTMENT OF CHEMISTRY

School of Natural Sciences

About Chemistry Department:

https://snu.edu.in/schools/school-of-natural-sciences/departments/department-of-chemistry/

Chemistry education at Shiv Nadar Institution of Eminence establishes a connection between the fundamental principles governing the nature of the universe and the science of life, spanning both traditional and various interdisciplinary areas. Chemistry, often referred as the central science, plays a vital role in nearly every other scientific field.

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

- Contribute to advancing and disseminating 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 in chemical and interdisciplinary projects.
- Train undergraduate, graduate students, and research fellows to become future independent scientists, serving the needs of society, academia, and industries.

Our vision is to create a positive impact on the world through cutting-edge research and innovation at Shiv Nadar Institution of Eminence.

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 an Integrated B.Sc.-M.Sc. (Research) degree for 5 years, Integrated B.Sc.-M.Sc.-Ph.D. for 9 years, Integrated M.Sc.-Ph.D. for 6 years, M.Sc. (Research) for 2 years and Ph.D. for 5 years.

Post-Graduate Courses:

The chemistry postgraduate (PG) courses are meticulously designed to enable students to advance their knowledge in the fundamentals of chemistry, including organic, inorganic, physical, and analytical chemistry. Simultaneously, the curriculum encourages students to correlate this knowledge at various interfaces. Computational aspects and relevant applications are integrated to strengthen the acquired knowledge further. The program provides many elective courses, allowing students to tailor their education to align with future opportunities. Foundation courses in the first semester ensure that all students have the necessary background to complete the course of study and fully benefit from the program. Well-equipped research labs offer an excellent platform for students to enhance their research skills, develop the ability to write research proposals, gain research exposure through in-depth dissertations supervised by a research advisor, and improve their capability to present scientific findings. This includes literature seminars, presentation skills, and a public thesis defense. The chemistry department provides a flexible and comprehensive curriculum that systematically prepares students for careers in chemistry and related fields upon graduation and helps them acquire leadership qualities.

Eligibility for Post-Graduate Programs:

Eligibility for the Ph.D. program requires students to have a minimum of 60% in M.Sc. in natural sciences. For the Integrated M.Sc.-Ph.D. and M.Sc. (Research) programs, students with a CGPA equivalent to 60% marks in a 3-year B.Sc. in Chemistry are eligible to apply. In the first two semesters, major courses ensure that students acquire both basic and advanced knowledge in requisite areas, including inorganic, organic, and physical chemistry. The postgraduate programs aim to instill innovative thinking skills in students, preparing them with both essential and advanced skills for better prospects in the future. This readiness is crucial for contributing to a sustainable world and adaptability in the ever-changing job market. Such goals are achievable with the support of our outstanding faculty, internationally renowned for their expertise in education.

Chemistry Careers:

The Chemistry program at SNIoE provides excellent career opportunities for Ph.D., post-doctoral fellowships, and employment in both industry and academia, both within India and internationally, including the US, Europe, Japan, Australia, and other regions. Major employment sectors include industries related to agricultural technology, biotechnology, pharmaceuticals, materials, and their applications. Additionally, chemists may explore job opportunities in various other sectors, including the chemical industry, and can advance their careers in forensic science, food science, and healthcare professions.

Chemistry Research at SNIoE:

Research activities at SNIoE extend beyond the postgraduate level, integrating with the undergraduate program through various lab-related components and possibly using the Research Experiential & Applied Learning (REAL) course platform. Undergraduate research is designed to help students realize and reinforce their chemistry knowledge obtained from formal coursework. It also plays a crucial role in developing their scientific and professional skills, fostering insight for addressing out-of-the-box questions. Original research projects, culminating in comprehensive written reports, offer an effective pedagogical approach to integrate undergraduate learning experiences. This approach allows students to participate in the learning process actively. Opportunities for research in chemistry at SNU are available in the following broad areas:

- Asymmetric Catalysis
- Bio-Inorganic Chemistry
- Catalysis
- Chemical Biology
- Chemical & Biological Crystallography
- Computational Quantum Chemistry
- Coordination Chemistry
- Electrochemistry
- Green Chemistry
- Materials Chemistry
- Sustainable Main Group Catalysis
- Medicinal Chemistry
- Metalloradical Chemistry
- Nano-biotechnology
- Physical Chemistry
- Polymer Chemistry
- Protein Chemistry
- Supramolecular Chemistry
- Synthetic Organic Chemistry
- Ultrafast Spectroscopy
- Materials for Environment
- Natural Product Synthesis

For specific research areas, please visit here: https://snu.edu.in/schools/school-of-natural-sciences/departments/department-of-chemistry/ (it same to departmental webpage)

Major in Post-Graduate Chemistry:

The Chemistry department at SNIoE offers a range of postgraduate chemistry courses to establish a connection between the fundamental principles of chemistry, interdisciplinary sciences, and their application at the research level. Every chemistry postgraduate student at 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**.

- **83 credits** = 33 credits (Chemistry Core Courses) + 25 credit (Chemistry elective courses) + 24 credits (Master project) + 1 credits Seminar (CHY615).

The credit requirements for **Integrated M.Sc.-Ph.D. in Chemistry** are **83 credits.**

- **83 credits** = 33 credits (Chemistry Core Courses) + 25 credits (Chemistry elective courses) + 24 credits (Master project) + 1 credit Seminar (CHY615).

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

- **211** credits = 128 credits from 3 years B.Sc. (as suggested in UG prospectus) + 83 credits from 2 years **M.Sc. (Research)**.

The credit requirements for **Integrated B.Sc.-M.Sc.-Ph.D. in Chemistry** are **211** credits.

- **211** credits = 128 credits from 3 years B.Sc. (as suggested in UG prospectus) + 83 credits from 2 years **M.Sc. (Research)**.

The credit requirements for **Ph.D. in Chemistry** are **12** Credits.

- **12** Credits = 6 credits (Chemistry Core/Major Courses including CHY615, CHY600, CHY512) + 6 credits (Chemistry elective courses).

Major courses in Post-graduate Chemistry

Semester	Course	Course Title	L :T : P	Credits
1 (MSN)	CHY512	Advanced Molecular Spectroscopy[$, ##]	3:0:0	3
	CHY527	Organic Reaction Mechanisms -1 [##]	2:1:1***	4
	CHY615	Graduate Seminar[$] (required and get 1 credit) [##]	1:0:0	1
	CHY649	Analytical Chemistry [##]	3:0:1**	4
	CHY511	Quantum Chemistry (Electives)	3:0:1	4
	CHY545	Fundamentals of Crystallography (Electives)	2:0:1	3
	CHY571	Materials for Energy (Electives)	3:0:0	3
	CHY504	Applications of Analytical Techniques (Electives)	3:0:0	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
	CHY542	Supramolecular Chemistry (Electives)	3:0:0	3
	CHY501	Medicinal Chemistry of organic molecules (Electives)	3:0:0	3
	CHY522	Cheminformatics for Drug and Materials Design (Electives)	2:0:3	3
	CHY544	Nanotechnology and nanomaterials (Electives)	3:0:0	3
	CHY616	Statistical Mechanics (Electives)	3:0:0	3
	CHY652	Advanced Biochemistry (Electives)	3:0:0	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
	CHY553	Coordination & Bio-inorganic Chemistry (Electives)	3:0:0	3
	CHY552	Polymer Chemistry and its Scope (Electives)	3:0:0	3
	CHY556	Inorganic reaction mechanism (Electives)	3:0:0	3
	CHY609	Strategies for problem solving (Electives)	3:0:0	3
	CHY621	Organic Named Reactions II (Electives)	3:0:0	3
	CHY642	Supramolecular Self-assembly and Functional materials (Electives)	3:0:0	3
	CHY697	Master Project [##]	0:0:6	6
3 (MSN): Total credits: 21				
	CHY644	Chemistry of Materials [##]	3:0:0	3

4 (SPR)	CHY899	Seminar*	1:0:0	0
	CHY601	Quantitative methods (Elective)	1:0:0	1
	CHY698	Master Project ##	0:0:6	6
		xxxxxxxxxxx		
4 (SPR): Total credits: 13				
Total Credits				**83**

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

Elective courses:

Course Code	COURSE NAME	L:T: P	Credits
CHY501	Medicinal Chemistry of Organic Molecules	3:0:0	3
CHY502	Synthetic organic Chemistry	3:0:0	3
CHY504	Synthetic organic Chemistry	3:0:0	3
CHY511	Quantum chemistry	3:0:1***	4
CHY522	Cheminformatics for Drug and Materials Design	2:0:1	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
CHY571	Materials for energy	3:0:0	3
CHY 601	Quantitative Methods	1:0:0	1
CHY609	Strategies for problem solving	3:0:0	3
CHY611	LASER spectroscopy	3:0:0	3
CHY616	Statistical Mechanics	3:0:0	3

CHY619	Advanced Quantum Chemistry	3:0:0	3
CHY621	Organic Named Reactions II	3:0:0	3
CHY627	Organic Reaction Mechanisms –II	3:0:0	3
CHY642	Supramolecular Self-assembly and Functional Materials	3:0:0	3
CHY644	Chemistry of Materials	3:0:0	3
CHY652	Advanced Biochemistry	3:0:0	3
CHY899	Graduate Seminar	1:0:0	1

** Practical of 2 hours; *** Practical 3 hours,

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

This course will provide the basic understanding of drug discovery from the perspective of how small molecules interact with the enzymes, receptors and proteins in the human body. These biomacromolecules are responsible to catalyze myriad bodily functions. We will discuss about the fundamentals of such interactions. We will also discuss the concept of medicinal chemistry and drug development.

Course Content:

Introduction and history of drug discovery	What is a drug or a pharmaceutically relevant candidate? How the concept of drug evolved over time and the interesting incidents associated with this discovery as well as the discoverer
Overview of modern rational drug design	How the modern-day drug discovery works, what is the process and how the process evolved over time and how it is different from the conventional way of discovery drugs. We will discuss about rational drug design and their advantages and disadvantages.
Drug Development	What is drug development? What are its individual components like medicinal chemistry, assay development, in vivo studies, pk/ pd, process research and formulation. How are these associated to each other?
Lead discovery	Definition of lead discovery. The procedures to discover leads such as high throughput screening, molecular modelling, fragment-based approaches, drug repurposing, natural product inspired drug discovery etc.

Lead modification	How to modify a drug from a lead to a hit molecule? What is a hit molecule? What are the aspects of such modifications? What the process such as structure activity relationship studies and etc., that are involved in such modifications.
Drug receptor interaction	Thorough interaction on what are receptors, their roles and repercussions. How drugs interact with the receptors and how these interactions could be modified and improved for better modulations.
Enzyme and enzyme catalysis in drug discovery	Definition of an enzyme, their roles and how these enzymes catalyze important chemical reactions in a human body which in turn evokes various physiological responses.

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

The CHY 502 "Synthetic Organic Chemistry" course is designed for students in the integrated BS-MS and integrated M.Sc.-Ph.D. programs. The central part of the course consists of an overview of some important classes of reactions with particular emphasis on mechanistic understanding and justification of observed selectivity when appropriate. This course aims to provide a comprehensive knowledge of various C-C, C=C, and C-heteroatom bond-forming reactions and their application in the synthesis of organic molecules. In addition, this course will help students to understand the logic, strategies, and tactics involved in complex molecule synthesis. At the end of the course, the student should be able to recognize the main structural features of a synthetic target and find a reasonable synthetic solution. The course consists of five units.

- **Unit 1**: Focuses on the chemistry of carbocations, nitrenes, and carbenes.
- **Unit 2** Focuses on the chemistry of carbanion, emphasizing the preparation of stereoselective enolates and their application to stereoselective C-C bond-forming reactions.
- **Unit 3**: Focuses on the different methods for the stereoselective synthesis of olefins (C=C). In this unit, the next focus will be on metathesis reactions and their application in organic synthesis.
- **Unit 4**: Focus on various cross-coupling reactions for the formation of C-C and C-N bonds and their applications in organic synthesis.
- **Unit 5**: Contains the logic, tactics, and planning of organic synthesis.

Course content

Chemistry of carbocations, carbenes,	Introduction of different types of carbocations. Various reactions of carbocation such as 1,2-hydride shift, 1,2-alkyl or aryl shift, pinacol-

and nitrenes,	pinacolone & semi-pinacol rearrangements, Dienone-phenol rearrangement, Rupe rearrangement. Introduction and classification of carbenes, methods for the preparation of carbenes, addition and insertion reactions of carbene, metal carbenoids and their use in organic synthesis. Introduction of nitrene, methods for the generation of nitrene intermediates, reactions of nitrene and related electron-deficient nitrogen intermediates, and rearrangement reactions of nitrenes.
Chemistry of Carbanion	Enolate structure & stereocontrolled generation of enolates, alkylation of enolates: reactivity *vs* selectivity, O vs C alkylation, the chemistry of chiral enolate, chirality appended with auxiliaries, Meyers bicyclic lactams, Seebach's self-reproduction chirality, and Evan's prolinol amide.
Olefination Reactions	Wittig reaction, Schlosser modification, Horner-Wadsworth-Emmons reaction, Julia-Lythgoe, Peterson reaction, Tebbe-Petasis, McMurry, Takai, and Ramberg-Bäcklund reaction. Introduction of metathesis reaction, classification, details mechanism, and usefulness in organic synthesis. *E*-Selective olefin metathesis reaction. *Z*-Selective olefin metathesis reaction.
Metal-mediated Cross-Coupling Reactions	Heck coupling reaction, Suzuki coupling reaction, Stille coupling reaction, Sonogashira reaction, Ullmann reaction, Tsuji-Trost reaction, Negishi reaction, Fukuyama reaction, Buchwald-Hartwig coupling.
Tactics of Organic Synthesis	Introduction to retrosynthetic analysis, disconnection guidelines for compounds with different functional groups. Disconnection strategy for three, four, five, and six-member ring skeleton. Disconnection of spiro and fused ring skeleton. Use of retrosynthetic analysis toolbox in complex natural product synthesis. Concepts of total synthesis, formal total synthesis, lineal synthesis, convergent synthesis, divergent synthesis, and their examples.

CHY504: Applications of Analytical Techniques (L : T : P = 3 : 0 : 0) (Elective Course)

The various spectroscopic techniques including UV-Vis, IR, ^{1}H NMR, ^{13}C NMR are used in conjunction with more advanced 2D NMR methodologies to determine structures of complex molecules. The focus of this course is 2D NMR spectroscopy and how it can be used together with 1D NMR and other spectroscopic methods mentioned above to determine structures of unknown compounds.

Course content

Topics	Contents
Introduction	General introduction, Calculating double bond equivalents (amount of unsaturation in a compound) from their molecular formulae. This is the first step to structure determination of an unknown compound.
NMR spectroscopy	Basic principal of NMR, Multinuclei 1D-NMR spectroscopy, chemical shift variation, identifying peak positions, calculating intensity and correlation with number of protons in ^{1}H-NMR, ^{13}C-DEPT analysis, complete assignment of peaks of organic and inorganic compounds. Introduction of 2D NMR spectroscopy and their application in solving solution structures. Homonuclear through-bond correlation 2D NMR (COSY, TOCSY), Heteronuclear through-bond correlation 2D NMR (HSQC, HMBC), Through-space correlation 2D NMR (NOESY, ROESY),
Application of NMR spectroscopy	Conformational analysis, Host-guest binding analysis, estimation of association constants, variable temperature NMR, estimation of thermodynamical parameters, estimation of activation energy of a reaction, estimation of enantiomeric excess, following progress of a chemical reaction, Fluxionality Analysis of inorganic compounds, and other relevant applications.
UV-vis spectroscopy	Basic principle and method, calibration plot, estimation of concentration of unknown solution, estimation of rate of a reaction, understanding of molecular association, Host-guest interaction, estimation of association constant and stoichiometry of an association (JOB's plot), etc.
Chromatography Methods	Introduction, paper chromatography, thin layer chromatography, column chromatography, high performance liquid chromatography (HPLC), estimation of purity of a sample, size exclusion chromatography, estimation of molecular weight of macromolecules.
Problem solving	Solving unknown structures using above spectroscopic techniques.

511: Quantum Chemistry (L : T : P = 3 : 0 : 1) (Elective Course for outside SNIoE)

The course offers fundamentals and basics of quantum chemistry. We discuss the basic postulates of the quantum mechanism, its foundation, and its applications to the hydrogen atom and other systems relevant to chemistry students. 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

Origin of Quantum Mechanics	Black body radiation, photoelectric effects, wave-particle duality, de Broglic equation, Heisenberg Uncertainty relations (without proof).
Postulates and General Principles of Quantum Mechanics	Basic concepts and properties of operators, eigen functions and eigen values, linear and non-linear operators, commutation of operators and commutator, expectation value, properties of Hermitian operators, postulates of quantum mechanics, Schrodinger equation, wave functions, acceptable wave functions, probability interpretations of the wave functions.
Particle in a One-Dimensional Box	Setting up Schrodinger equation for particle in a one-dimensional box, solution of Schrodinger equation, energy eigen values and wave functions, properties of wave functions (normalization, orthogonality, probability distribution), expectation values of x, x^2, p_x and p^2_x and uncertainty principle, particle in two and three dimensional boxes, degenerate energy levels, Concept of quantum tunnelling.
Quantized Vibrational Motion	Setting up of Schrödinger equation for simple harmonic oscillator (detailed solution is not required), discussion of eigen values and wave functions, vibrational selection rule.
Quantized Rotational Motion	Quantization of angular momentum, rigid rotator model for diatomic molecule, Schrödinger equation, energy and wave functions (no derivation), coordinate transformation, Spherical Harmonics.

Hydrogen Atom	Schrödinger equation in Spherical polar coordinates, radial part, radial wave function (no derivation), probability density, radial distribution function, quantization of energy (only final energy expression).
Molecular Orbital Theory	LCAO treatment of H2+, bonding and antibonding MOs, qualitative LCAO treatment of H2 (detailed derivation not required), Basic concepts of HF and DFT.

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

This course covers rotational, vibrational, Raman, UV-Visible, fluorescence, and NMR spectroscopy methods. Group theory will be utilized to explain the spectroscopic selection rules. Chemical and biochemical systems are often analyzed using these techniques to identify their electronic and molecular structures. During this course, students will acquire an understanding of the behavior of molecular systems under different electromagnetic fields. Each spectroscopy method will be discussed regarding its principles, sufficient theories, and applications.

Course content

Rotational spectroscopy	Introduction and review, Rotational spectroscopy of diatomic rigid and non-rigid molecules, Symmetric top and spherical top molecules, Asymmetric molecules
Vibrational spectroscopy (Infrared)	Energy of harmonic oscillator, Morse potential and anharmonic oscillator, Infrared spectroscopy, Vibrating rotator, Breakdown of Born-Oppenheimer approximation, 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, Hyperpolarizability, Rotational Raman spectra, Vibrational Raman spectra, Rule of mutual exclusion.

UV-Vis absorption and Fluorescence spectroscopy	Theory of UV-Vis spectroscopy, Born-Oppenheimer Approximation and molecular potential energy curve, Molecular term symbol, Selection rules, Franck-Condon principle, Franck-Condon factor, Spin-orbit coupling, Jablonski diagram, Fluorescence and phosphorescence, Vibrational relaxation, Non-radiative and radiative processes, Internal conversion and intersystem crossing, Stokes Shift and solvent effect, Fluorescence lifetime, Quantum yield, Fluorescence quenching and Stern-Volmer equation, Static and dynamic quenching.
Nuclear Magnetic Resonance (NMR)	Nuclear spin, 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, Pulse techniques in NMR, Rotating frame of reference, Spin-spin relaxation and spin-lattice relaxation, Fourier Transform NMR, Nuclear Overhauser effect (NOE), Concept of 2-dimensional NMR spectroscopy (2D COSY and 2D TOCSY)
Group Theoretical treatment of selection rules	Symmetry elements and symmetry operations, Point groups, Reducible and irreducible representations, Character tables, Symmetry-adapted linear combination (SALC), Spectroscopic selection rules

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

In this course, various techniques for studying very fast chemical reactions, basic statistical thermodynamics, 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. During this course, students will acquire an understanding of the connection between macroscopic chemical kinetics and microscopic reaction dynamics. This course covers a range of lab experiments, from reaction rates to thermodynamic properties.

Course content

Classical thermodynamics	Revisit of first and second laws of thermodynamics, Nernst heat theorem, and third law of thermodynamics
Statistical thermodynamics	Phase cell, Concept of various ensembles, Thermodynamical probability and entropy, Boltzmann statistics, Concept of Fermi-Dirac and Bose-Einstein statistics, Molecular partition functions, Translational, rotational, vibrational and electronic contribution to the molecular partition function and molecular energy, Canonical partition function, Mean energy, Internal energy, Heat capacity, Entropy, Boltzmann entropy formula, contribution of various modes of motion to entropy, Residual entropy, Enthalpy, Helmholtz energy, Gibbs energy, Equilibrium constant, Relation between equilibrium Constant to state populations
Kinetics of fast reaction	Kinetics of fast reaction, stopped-flow and relaxation methods for rate measurement, flash photolysis, temperature-Jump method
Reaction dynamics	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, 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), Electron transfer reaction and Marcus theory, Reaction in molecular beams, Features of potential-energy surfaces, State-to-state kinetics, Effect of vibrational and rotational energy on reaction rate, Study of transition state species. Spectroscopic observation of chemical reaction dynamics.
Practicals	Determination of rate constant of chemical reactions, Influence of ionic strength on reaction rate, Determination of thermodynamic and kinetic properties of some chemical reaction from spectroscopic observables (peak frequency, amplitude and fwhm), Cyclic voltammetric study of some chemical systems.

CHY522: Cheminformatics for Drug and Materials Design (L : T : P = 2 : 0 : 1) (Elective Course)

This course and the associated computer lab deal with Cheminformatics and Bioinformatics, applied to the search for new drugs with specific physiological effects (*in silico* Drug Discovery) and new materials with specific properties. Students will learn the general principles of structure-activity relationship modeling, docking and scoring, homology modeling, statistical learning methods, machine learning, deep learning and advanced data analysis. They will gain familiarity with software for structure-based and ligand-based drug discovery. At the end of the course, students will be expected to present a completed piece of software of significant utility, OR an analysis of experimental data from their own work or from the published literature. Students will be encouraged to seek avenues for publication of their most significant results.

Course Content

Introduction	• Drug Discovery in the Information-rich age. • Introduction to Pattern recognition and Machine Learning. • Supervised and unsupervised learning paradigms and examples. • Applications potential of Machine learning in Chem- & Bioinformatics. • Introduction to Classification and Regression methods. • Types of classification and regression.
Representation of Chemical and Biochemical Structures	• Sequence Descriptors • Text mining • Representations of Molecular Structures • Characterizing 2D structures with Descriptors and Fingerprints • Searching 2D Chemical Databases • Chemical File Formats: SMILES and SMARTS • Graph Theory and Topological Indices • Substructural Descriptors • Molecular Fingerprints • Physicochemical Descriptors • Descriptors from Biological Assays • Representation and characterization of 3D Molecular Structures • Calculation of Structure Descriptors • Pharmacophores • Molecular Interaction Field Based Models • Local Molecular Surface Property Descriptors • Quantum Chemical Descriptors • Shape Descriptors • Protein Shape Comparisons

	• 3D Motif Models • Representation of Chemical Reactions and Databases
Analysis and Visualization	• Molecular Similarity Analysis • Molecular Quantum Similarity Measures • Cluster and Diversity analysis • Network graphs from Molecular Similarity • 3D visualization tools • Self-Organized Maps • Semantic technologies and Linked Data
Mapping Structure to Response: Predictive Modeling	• Linear Free Energy Relationships • Quantitative Structure-Activity Relationships (QSAR) Modeling • Ligand-Based and Structure-Based Virtual High Throughput Screening • 3D Methods - Pharmacophore Modeling and alignment • ADMET Models • Activity Cliffs • Structure Based Methods, docking and scoring • Site Similarity Approaches and Chemogenomics • Model Domain of Applicability assessment
Data Mining and Statistical Methods	• Linear and Non-Linear Models • Feature selection • Partial Least-Squares Regression • Introduction to Neural Nets, Bayesian Methods and Kernel Methods • Support vector machines classification and regression, and application to cheminformatics & bioinformatics • Random forest Principal Component analysis and SVD • Data preprocessing and different performance measures in Classification & Regression • Genetic Algorithms • KNN and Linear Discriminant analysis • Introduction to evolutionary computing • Deep Learning and Convolutional Neural Nets • Data Fusion • Model Validation • Interpretation of Statistical Models • Best Practices in Predictive Cheminformatics

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 Alkaloids and classification	Definition, structure and classification of alkaloids, Proposed biosynthesis of alkaloids, alkaloids and plants chemical defense mechanism
Chemistry of indole alkaloids and benzoisoquinoline alkaloids	Chemistry of indole alkaloids & 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 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 jatropholones synthesis of cembrene
Application of the Chemistry terpenoids in Modern Medicine and Fragrance	Story of Taxol & 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)

In this course, various mechanistic aspects of organic reaction will be discussed. 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. Application of these mechanistic parameters as well as experimental tools will 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. 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.

Postulates and principles of kinetic analysis	Hammond postulate and the Curtin-Hammet principle; Microscopic reversibility & Kinetic vs Thermodynamic control, and its application in studying reaction mechanism
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 and its application in studying reaction mechanism.
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, and its application in studying reaction mechanism.
Thermochemistry of reactive intermediates	Stability versus persistence & chemistry of carbanions, chemistry of classical and non-classical carbocations.
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.
Molecular symmetry and chirality	Symmetry operations and symmetry elements, point group classifications and symmetry numbers.
Dynamic stereochemistry: Stereoselective reactions	Stereoselectivity: Classification, terminology, and principle, stereo-selection in cyclic and acyclic systems (Cram's & Felkin-Ahn Model) and their application.
Chirality in molecule devoid of chiral centers	Stereochemistry of allenes, spiranes, propellers and gears, Stereochemistry of helicenes and molecules with plane of chirality,
General and characterization of	Historical background, long-lived free radicals and detection of free radicals, structure, stereochemical properties and substitution

free radicals and radical intermediates.	effects, general features of free radicals, kinetics characterization of chain reactions, determination of reaction rate and structure-reactivity relationships.
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.
Other types of free radical reactions	Halogen, sulfur, and selenium group-transfer reactions, intramolecular hydrogen atom transfer reactions and rearrangement reactions of free radicals.
Academic Week	Experiments
	Introduction to the lab notebook requirements and grading
	E1. Grignard Synthesis of Triphenylmethanol.
	E2. Grignard Synthesis of Triphenylmethanol cont.
	E3. Wittig olefination Reaction.
	E4. Wittig olefination Reaction cont.
	E5. Friedel-Crafts Acylation Reaction.
	Mid-term Examination
	E6. Friedel-Crafts Acylation Reaction cont.
	Make up week/viva.
	E7. Jones Oxidation reaction
	E8. Jones Oxidation reaction cont.
	E9. Synthesis of ibuprofen.
	E10. Synthesis of ibuprofen cont.
	E11. Synthesis of ibuprofen cont.
	Make up week /Viva

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: Chemistry of artificial receptors will be discussed with the help of some important recent literatures to keep this course up to date.

Course Content

Introduction Noncovalent interactions	Ion pairing, Ion-Dipole Interactions, Dipole-Dipole interactions, Dipole-Induced Dipole and Ion-Induced Dipole interactions, Hydrogen bonding (definition, structure and stability, strength, Halogen bonding, Cation-interactions, Anion-p interactions, p•••p interactions, Hydrophobic effect.
Aromatic-Aromatic Interactions	Benzene crystals, edge-to-face vs. face-to-face stacking interactions, N-H•••p interactions, sulfur-aromatic interactions, Benzene hexafluoro-benzene p-stacking.
Supramolecular Host-guest chemistry	Receptors, Lock and Key analogy, Binding constant analysis
Artificial Receptors	a) Cation Binding Hosts Podand, Crown Ether, Cryptand, Calixarenes. Their Nomenclature and Selectivity, b) Anion binding hosts: Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts. c) Ion pair receptors d) Hosts for Neutral Receptors: Clathrates, Inclusion Compounds, Guest Binding by Cavitands and Cyclodextrins, cucurbituril.
Supramolecular catalysis and reaction in confined environment	Definition, H-bonded cages for catalysis, Self-assembling coordination cages and their uses in encapsulations and catalysis, Phase transfer catalysis
Supramolecular Chemistry in Biology	Frist principle of self-assembly, Membranes, Macrocyclic systems, Photosynthesis, Oxygen transport, Enzymes, Heme analogues.

Biological supramolecular systems	Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly.
Supramolecular interactions in polymers	Metal Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), characterization, applications

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

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

Basic understanding of Materials	✓ Introduction: Fundamental study of materials in nanosize domain, history of nanomaterials ✓ Bulk Vs. Nanomaterials, Different types of nanomaterials based on their dimension (Carbon nano-architectures: carbon materials: Fullerene, SWNT, MWNT, Graphene, nanodiamonds, etc.) ✓ Quantum confinement effect ✓ Size effect over bonding, surface energy, mechanical, thermal, optical, magnetic, electrical and electronic properties. ✓ Nanostructures of silicon and other materials such as germanene, phosphorene, MoS_2, borophene, etc. ✓ Morphology effect over electronic and catalytic properties
Materials Synthesis Methods	✓ Methods of preparation of nanomaterials, physical methods and chemical methods ✓ ***Nanomaterial's synthesis***: Top down and Bottom-up approaches, Physical and chemical methods, Nucleation and growth of nano systems; self-assembly,

	✓ Synthesis of various materials with examples including ZnO nanoparticles; TiO2 nanostructures, AuNR, etc. Biological methods (Green synthesis Using microbes and plants).
Characterization Techniques	✓ ***Characterization of nanomaterials***: Spectroscopic/Optical methods; UV-VIS, Dynamic Light Scattering; (DLS), Raman, IR, XRD, Particle; Microscopic characterization: SEM, TEM, AFM.
Materials Applications	***Applications of nanomaterials and nanotechnology:*** Nano-machines, solar cells, coatings, MEMS, nanomedicine, sensors, magnetic storage devices, miscellaneous. Brief applications on drug delivery and diagnostics.

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 topics such as symmetry in crystallography, crystal 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. It will include hands-on training on crystal growth, mounting, structure solution, refinement, and analysis. Further, training on database use 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, Xray 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, ∆F synthesis.
Refinement of Crystal Structures	Refinement by Fourier synthesis, refinement by ∆F 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 (Few initial practical classes will be converted to tutorials)	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)

This course aims 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. Recent literature on f-block elements will be discussed in class.

Course content

Introduction	Sources of elements, “f” orbitals, oxidation states, atom and ion sizes, lanthanoid contraction, isolation and purification of uranium from natural source, separation using cation exchange resin, properties of the elements, general trends, binary compounds (oxides and halides of lathanides and actinides)
Coordination and organometallic chemistry	Coordination complexes of f-block elements, aqueous and redox chemistry, organometallic compounds of uranium, transuranium and transactinium elements, σ-bonded organometallic complexes, cyclopentadienyl complexes, arene complexes
Spectroscopic and magnetic properties	“f-f” spectra of lanthanides and actinides, luminescence property, bonding parameters and structural evidence 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, organocerium reagents, catalysis by lanthanide alkoxides, smoke detection.

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

This course will teach advances in inorganic chemistry, including learning the concept of physical inorganic chemistry using a molecular orbital approach, spectroscopy, and reaction kinetics to provide a deep understanding of various inorganic chemistry topics. A special emphasis on the chemistry of rings, clusters, and cages will be provided. Finally, recent progress in photochemistry and photochemical processes will be discussed. This course is also complemented with futuristic laboratory experiments, which will help students learn advanced laboratory techniques. Therefore, it would help their future research endeavors.

Course Content

Bonding theories and d-d transition	Crystal Field Theory (CFT), Ligand Field Theory (LFT), Molecular Orbital Theory (MOT), Metal-centered electronic spectra of transition metal complexes: microstates, determination of ground and all excited state terms of dn ions, splitting of dn terms in octahedral and tetrahedral fields, Orgel diagrams, qualitative idea of Tanabe-Sugano diagrams, charge transfer spectra according to MO theory.
Metal-metal bonding	Metal-metal bonding (M.O. concept), metal-metal bonded dinuclear complexes-typical examples, metal-metal multiple bonds, Bonding in dirhenium complexes, d* ¬ d transition.
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. Coupling between paramagnetic centers, Ferromagnetism, Antiferromagnetism, Ferrimagnetism, concept of single Molecular Magnet (SMM).
Wade's rules	Wade's rules, Carboranes, Metalloboranes. Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, capping rules.
Stereoisomers in coordination chemistry	Linkage isomers, stereo isomerism, cis, trans-isomers, interconversions, fac and mer-isomerization, Ray-Dutt twist, Bailar twist, trans directing ligands, trans-effect.
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.
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.
Practical (3 h)	a. Rhodium Rainbow: ligand field effects of dirhodium tetraacetate. b. Determination of Δ0 in Cr(III) complexes and spectrochemical series. c. The synthesis and characterization of Ferrocene and its derivatives. d. Synthesis of compound containing Metal-Metal Quadrupole Bonds and assignment of d* ¬ d transition. e. Synthesis of a selected Metal-organic Framework (MOF) and characterization. f. Preparation of trans-dichloro-bis(ethylenediamine)cobalt(III) chloride and cis-trans interconversion. g. Synthesis, Optical Resolution of $Co(en)_3^{3+}$. h. The Preparation of tetraphenylporphyrin and its Metal Complex, comparison of molar extinction coefficient. i. Preparation and Analysis of Potassium Trisoxalatoferrate(III) Trihydrate and photochemistry. j. NMR Investigation of Molecular Fluxionality: Synthesis of Allylpalladium Complexes.

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 for 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 an 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

Introduction	Meaning of coordination chemistry and use of metal coordination in both materials and biological sciences
Structure and bonding,	Bonding of organic ligands to transition metals, Octahedral vs Trigonal

spectroscopy	Prismatic coordination geometry, T-shaped complexes, π-bonding, electronic spectra based on metal to ligand. (example from various Journal Publications)
Stability of complex	18 electron rule, Statistical and non-statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes, redox stability
Magnetism	First order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes in cubic and axially symmetric crystal fields, low spin-high spin crossover
Recent development of coordination compounds and their use	Metal coordinated cage compounds-applications, catalysis for organic transformation, energy harvesting, light-emitting diodes. (examples from various Journal Publications)
Exam 1	Exam will be based on the above materials taught in the class
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	What is Bioinorganic Chemistry? General terms, how and why does nature select inorganic elements? Inorganic Elements and evolution. Basic biological Coordination Chemistry. Kinetic and spectroscopic characteristics of bioinorganic systems, coordination chemistry of non-redox active metal centers to biological complexes. Systematic overview over tasks and examples of inorganic elements in biology.
Non-redox active metals	Ion transport: membranes, energy, channels, pumps, comprehend and discriminate the different mechanism developed to cross cellular boarders, biomineralization
Redox active metals	Oxygen transport – metal-oxygen coordination in proteins, Oxygen activation and processing by cytochromes

Electron transfer	Electron transport in biology – iron sulfur clusters, enzymes for respiration, photosynthesis and related pathways
Water splitting	Small molecule activation and conversion by metalloenzymes – photosynthetic water splitting, comprehend and discriminate the different mechanism of enzymatic dioxygen activation without cytochromes
Radical scavenging	Radicals and bioorganometallic chemistry – from RNA to DNA and from Vitamin B12 to methanogens and methanotrophs, explain, how nature creates and utilizes radical intermediates in enzyme mechanism
Hydrogen and Nitrogen activation	Biological conversion and formation of hydrogen and nitrogen– hydrogenases and nitrogenases, understand based on coordination chemistry principles, how nature tailors metal centers to activate hydrogen and nitrogen.
Medical Implication	Metal pharmacology: uptake storage toxicity, explain the principles and mechanism of, how homeostasis is retained in a cell, Metals in medicine: anti-cancer agents, diabetes, arthritis, radionuclides and related applications, know and understand medical applications of metal ions and complexes

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

Over the past decade, the scientific community, particularly in chemistry, has been actively working towards developing environmentally friendly chemistries to safeguard human health and the environment. While efforts have been made to protect nature and maintain ecological balance, these initiatives are still in their early stages. The question arises: Are we genuinely protecting the Earth? Are we using natural resources wisely? The hazards associated with missteps in this regard are significant.

Chemistry surrounds us from morning to night in various forms, from personal care products to household items. Those with an understanding of and engagement in chemistry have a responsibility to use it sustainably. With knowledge comes the duty to acknowledge and address the impact of the science we practice. A collective effort is needed to align both new and existing chemistries towards being more benign and safer for Mother Earth.

Course Content

Green chemistry	Learning from the past for a brighter future: Understanding needs, limitations, and opportunities. Exploring the principles of Green Chemistry, including concepts like Atom efficiency, E factors, homo vs. heterocatalysis, reaction efficiency, and toxicity reduction, with real-world examples.
Green reactions	Exploring green alternatives: Non-risky reagents, benign solvents (aqueous medium, ionic liquids, supercritical fluids, solvent-free reactions), and nonconventional energy sources (microwave, ultrasound, photochemical reactions). Catalysis options include heterogeneous, biocatalysis, and phase-transfer catalysis. Real-life cases highlight the replacement of non-green reactions with environmentally friendly alternatives.
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.

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 racemization, Ray-Dutta and Bailar twist mechanisms, inorganic substitution reaction for octahedral geometry vs. square planar geometry, trans effect vs. trans directed effect.
Electron transfer reactions	Franck-Condon principle, Outer sphere ET, Marcus Theory of electron transfer, Electron transfers in biological systems, Inner sphere ET, Proton coupled ET (PCET) in biological systems and artificial photosynthesis
Reactions of coordinated ligands	Insertion, One electron and two electron oxidative addition, Reductive elimination
Catalysis and electrocatalysis	Homogeneous and heterogeneous catalysis by metal complexes, catalytic cycles, industrially relevant catalytic processes and mechanism, electrocatalysis, reaction mechanism studies by electrochemistry

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

Recent advances in medicine have led to the design and development of numerous novel synthetic architectures for targeted drug delivery, aiming to revolutionize the treatment and prevention of diseases. Advanced drug delivery and targeting present notable advantages over conventional drugs, including enhanced efficiency, improved safety in drug delivery, and increased convenience. However, the realization of this potential is often hindered by significant obstacles to in vivo drug delivery. These challenges are so substantial that effective drug delivery and targeting are now acknowledged as essential for developing various therapeutics, including theranostics. This course offers a comprehensive introduction to various carriers for drug delivery, covering the principles of advanced drug delivery and targeting, their current applications, and potential future developments.

Course Content:

Introduction	Introduction to intelligent materials and structures

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:	Commercial sources, synthetic methods, capsules/vesicles, their methods of preparations such as emulsification, Layer-by-Layer assembly, coacervation and internal phase separation. Design of organic based DDSs (Inorganic nanoparticles) including, Polymer-based Amphiphilic Nanocarriers, Micelle and Vesicle Nanocarriers from Polymer-Based Amphiphiles, Poly(lactic Acid) (PLA), (PLGA) Copolymers, Chitosan, Temperature-Sensitive Polymeric Nanocarriers (Thermosensitive Poly(*N*-isopropylacrylamide) (PNIPAm), thermo-responsive (Pluronic), Polymeric Nanogels, Liposome nanocarriers and Dendrimers.
Nanotechnology in medicine: Nanoparticles in drug delivery:	Design of inorganic based DDSs (Inorganic nanoparticles) including, Carbon Nanotubes, Gold Nanoparticles (Au NPs), Quantum Dots (QDs), Superparamagnetic Iron-Oxide Nanoparticles (SPIONs), Mesoporous Silica Nanoparticles, Organic/Inorganic Hybrid Nanocarriers. Novel delivery modalities, including active targeting and passive targeting DDSs, advantages and disadvantages will be discussed.
Approaches for drug release	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). Physical and chemical triggering phenomena: Chemical triggers, pH-responsive materials, biologically induced reactions, thermally induced release/ temperature responsive, electrical, magnetically initiated triggering.
Toxicity of metallic	Is it safe for metal-based nanoparticles for medicinal applications?

nanoparticles and Applications of nanomaterials to biology or medicine	Cancer therapy (Thermal therapy); Diagnostic testing.

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 *etc*., 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 complexes	Substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. 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

CHY571: Materials for Energy (L : T : P = 3 : 0 : 0) (Elective Course)

The research focuses on establishing a fundamental understanding of the structure-composition-performance relationships in energy materials. The primary objectives involve the fabrication and evaluation of prototype clean energy conversion and storage devices, including lithium batteries, perovskite-based solar cells, supercapacitors, and fuel cells.

Course Content

Topics	Contents
Basics of Inorganic functional materials	Inorganic nanomaterials and quantum dots, Metal oxides (0D, 1D, 2D and 3D), Carbon nanomaterials (quantum dots), Porous carbon and graphene.
Fundamental concepts in energy systems	Electrochemical Cell, Faraday's laws, Electrode Potentials, Thermodynamics of electrochemical cells, Polarization losses in electrochemical cells, Electrode process and kinetics, Electrical double layer, heterogeneous catalysis (Electrocatalysis).
Nanomaterials for energy conversion	Issues and challenges of functional nanostructured materials for electrochemical energy, Conversion systems, Fuel cells, Principles and nanomaterials design for; Proton exchange membrane fuel cells (PEMFC); Direct methanol fuel cells (DMFC); Solid-oxide fuel cells (SOFC), Current status and future trends
Nanomaterials for energy storage (Batteries)	Issues and challenges of functional nanostructured materials for electrochemical energy storage systems, Primary and secondary batteries (Lithium ion Batteries), Cathode and anode materials, Nanostructured carbon based materials, Novel hybrid electrode materials, Current status and future trends

Nanomaterials for energy storage (Capacitor).	Capacitor, electrochemical supercapacitors, electrical double layer model, Principles and materials design, Nanostructured carbon based materials, Redox capacitor Nano- oxides, Conducting polymers based materials, Current status and future trends.
Materials for other applications	Sensors and actuators, Nanomachines, Magnetic materials, Photonic materials, Superconductivity, Thermoelectric materials, Perovskites, Metal clusters, Piezoelectricity and active materials.

CHY600: Research Methodology (L : T : P = 2 : 0 : 0) (Core 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 skills, and scientific techniques. Classes will be through lectures, reading articles, and presentations. Students are expected to research literature, read articles, discuss, and present relevant articles to be supplied by the instructor(s) in class.

Introduction	Overview Lecture
Ethics, Academic dishonesty, plagiarism, Lab safety	An overview lecture on publication ethics, focusing on data fabrication and falsification, plagiarism, and improper author contribution, will be provided. The aim is to instill an understanding of the ethics involved in academic and research publications. Additionally, the importance of lab safety will be emphasized. The lecture will cover safety rules and regulations to create a safe working environment. Exploring these safety protocols improves awareness of potential hazards and mitigating risks associated with laboratory work.
Plan/design of experiments/Theory and Maintaining notebook	How students can plan for new research in the beginning of research career including M.Sc. research and Ph.D. Identifying the research 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.

CHY601: Quantitative Methods (L : T : P = 1 : 0 : 0) (Elective Course)

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.

Course Content:

- 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. Optimization of mathematical functions and root findings: minimizations and maximizations, fitting equations to data.

CHY609: Strategies for problem solving (L : T : P = 3 : 0 : 0) (Elective Course)

This course will teach problem-solving strategies through lectures, tutorials, and home assignments. The courses will provide a journey of various subjects learned and utilize them to approach and answer several problems. Physical chemistry syllabus will discuss several questions and answers, 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, problems in the inorganic syllabus will discuss 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. 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)

Statistical mechanics has influenced the understanding of the different macroscopic properties of materials in thermodynamic equilibrium by building the connection with the dynamical laws governing the microscopic constituents of the materials. It deals with the probabilistic understanding of the different thermodynamic ensembles, which form the basis of the interacting and non-interacting systems. This course will introduce the students to various ideas and concepts of statistical mechanics. The course contains basic aspects of statistical thermodynamics, understanding the probabilistic theorems to evaluate the thermodynamics properties, such as the internal energy, entropy, enthalpy, etc., of different statistical ensembles, and the properties of interacting and non-interacting systems.

Course content

Thermodynamics and Mechanics	Thermodynamic Equilibrium state, Laws of thermodynamics, Axiomatic formulation of thermodynamics, Thermodynamic potentials, Classical and Quantum Mechanics, Hamiltonians, Stirling's approximation, probability and statistical methods.
Ensembles in Statistical Mechanics:	Ensemble postulate and ergodicity, Ensemble averages, methods of most probable distributions, Micro-canonical, canonical and grand canonical ensembles, Quantum and classical partition functions, Phase space, Fluctuations, Thermodynamic connections.
Non-interacting systems	Factorization of the partition function, Occupation numbers, Collections of fermions, bosons and photons, Bose-Einstein Statistics, Classical ideal gas of spinless particles, molecular partition functions.
Chemical Equilibrium	Equilibrium constants in terms of partition functions, examples and calculations of equilibrium constants.
Interacting Systems.	Configurational Partition functions, Pair correlation function, Virial equation and Meyer cluster diagrams, Phase Transitions in Lattice models and Lattice gas, Ising Model.

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

Quantum chemistry offers a quantitative view of molecules and accurately predicts chemical and physical properties of molecules. This course will discuss the quantum mechanical treatment of molecular rotation, molecular vibration, and hydrogen atom, various approximation techniques, valance bond theory, and molecular orbital theory, various mean field theories, including Hartree-Fock self-consistent field and density functional theories, and exchange-correlation functional. A portion of the course will deal with time-dependent quantum mechanics.

Course content

Time-Independent Quantum Mechanics	Formalism of quantum mechanics Quantum mechanics of vibration and rotation Quantum mechanical hydrogen atom
Variation Method	Variation method, Secular determinant
Perturbation Theory	Time-independent perturbation theory Solution of time-dependent Schrodinger equation: Schrodinger, Heisenberg and Interaction Pictures Two-level systems Time-dependent perturbation theory, Fermis Golden rule
Mixed State and Density Matrix	Density matrices and density operator Bloch formalism Energy representation of the density operator: coherences
VB and MO Theories	Born-Oppenheimer approximation Electronic Schrodinger equation for molecules Valence bond method The molecular orbital theory Hückel approximation MO term symbols
Mean Field Theories	The Hartree-Fock self-consistent field method Electron correlation Density Functional Theory Exchange-correlation functional QM/MM formalism

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

The course CHY 621 “Named Organic Reaction II,” is designed for 2nd year M.Sc. and Ph.D. students. This course includes various important organic reactions to build complex organic molecules with an emphasis on symmetry-controlled transformations, photochemical reactions, and multicomponent reactions. Different pericyclic reactions and related fundamental principles will be taught in the first part of this course. Next, details of photochemical reactions and their application will be discussed. Afterward, numerous name reactions for functional group transformation will be covered. In the last part, the emphasis will be on several multicomponent reactions and their applications. This course will equip students with enough knowledge of various organic name reactions and their probable mechanisms to carry out multistep organic transformations.

The course is divided into four major units.

- **Unit 1**: Details of Pericyclic Reactions.
- **Unit 2**: Focuses on Photochemistry
- **Unit 3**: Focuses on Functional Group Transformation
- **Unit 4**: Focuses on Multicomponent, Tandem Reactions.

Course Content

Pericyclic Reactions	Introduction of pericyclic reaction, classification of pericyclic reactions, frontier molecular orbitals of polyene systems, and the different theories to analyze pericyclic reactions. Details of Electrocyclic reactions: stereospecificity of electrocyclic reactions, torquoselectivity of electrocyclic reaction, electrocyclic reaction of three-member ring systems, Nazarov cyclization, application of electrocyclic reaction in organic synthesis. Cycloaddition reaction; analysis of cycloaddition reaction using Woodward–Hoffmann symmetry correlation, FMO, PMO methods, details of [4+2], [2+2] cycloaddition, [1+3] dipolar cycloaddition reactions, application of cycloaddition reaction in organic synthesis. Sigmatropic Rearrangement; Details of [1,3], [1,5], [1,7], [3,3] sigmatropic rearrangements, Claisen rearrangement, Aza-Claisen rearrangement, Aza-Cope rearrangement, Anionic Oxy-Cope rearrangement, Overman rearrangement, Eschenmoser-Claisen rearrangement. Cheletropic reaction. Group transfer reaction.
▪ Photochemistry	Basic principles, Jablonski diagram, photochemistry of olefinic compounds, *cis-trans* isomerisation, Paterno Buchi reaction, Norrish type I and II reactions, quantum yields, photosensitization and energy transfer reactions, photo oxygenation and photo fragmentation, photochemistry of aromatic compounds, isomerisation, additions and substitutions, di-pi-methane rearrangement, Bartons reaction, Photo-Fries rearrangement.

▪ Functional Group Transformation	Baeyer-Villiger oxidation, Corey-Kim oxidation, Dess-Martin periodinane oxidation, Tamao-Kumada-Fleming oxidation, Rubottom oxidation, Swern oxidation, Wacker-Tsuji oxidation, Woodward cis-dihydroxylation, Luche reduction, Meerwein-Ponndorf-Verley reduction, Staudinger reaction, Mitsunobu Reaction Kolbe–Schmitt reaction, Arndt-Eistert synthesis, Hofmann–Löffler reaction, Barton Decarboxylation, Barton-Macombie Decarboxylation., She Epoxydation, Sharpless Dihydroxylation.
Multicomponent	Introduction of multicomponent reactions. Biginelli reaction, Passerini reaction, Ugi reaction, Petasis (Boronic Acid Mannich) reaction, Povarov reaction etc.

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 Alkyl C-H Bonds	Functionalization of aliphatic C-H Bonds by Carbene Insertions. 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	Borylation and silylation of aromatic C-H bonds. Alkylative

bond activations and functionalization, Aromatic C-H Bonds	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.

CHY642: Supramolecular Self-assembly and Functional Materials (L : T : P = 3 : 0 : 0) (Elective Course)

This is an advanced interdisciplinary course combining both supramolecular and materials chemistry. This course will cover the recent trends of material chemistry and functional materials. This course aims to teach fundamental aspects of the self-assembly process, including biomacromolecular self-assembly, which is the basis of every living organism. This self-replication phenomenon is responsible for the evolution of life. Moreover, dye aggregation and all underlying theorems, as well as thermodynamic and kinetic aspects that influence the aggregation process, will also be covered in this course. An introduction to a new, exciting class of polymers, namely supramolecular polymers, and their possible future applications will be covered in the course. Some important recent literatures will be discussed in the class to keep this course up to date.

Course content

Topics	**Contents**

Introduction	Noncovalent interactions, Hydrophobic effect, Frist principle of self - assembly, Self-replication and evolving systems, Concept of molecular motors and machines.
Dye aggregation	Principle of Dye aggregation, Photophysical behavior of aggregated systems, *H* and *J*-aggregates, Kasha Model, Modified Kasha Model
Thermodynamic and kinetic aspects of dye assembly	Thermodynamic aspects of Dye assembly, Structure-binding strength relationship, Solvent effect on aggregation, Dimers/Extended aggregates: Isodesmic vs. (anti-)cooperative self-assembly, General considerations of kinetic aspects, Merocyanine and Perylene bisimide systems.
Supramolecular polymers	Design principle, Polymers beyond conventional polymers, Living Supramolecular polymers, Supramolecular Block Copolymers, Characterizations, Examples and Applications
Out-of-equilibrium systems	Out-of-equilibrium self-assembly, Adaptive and fuel driven systems, System chemistry, evolution of life
Soft materials	Liquid crystals, Micelles, Reverse micelles, and Gels
Functional Materials and application	Color and fluorescence sensors, Molecular probe for life-sciences, Organic materials for photovoltaics, organic nanomaterials

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 advancing society and high technology development. It interfaces with chemistry, chemical engineering, life science, and materials science and, therefore, has an 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 properties, and design of optimal materials are emerging areas of materials research. The theoretical aspect and prediction of stable structures guide the experimental outputs and play a distinct role in dictating 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	X-ray diffraction, overview of Bravais lattices, crystal systems and symmetry in crystals, crystal defects, different types of bonding in materials.
Electronic, magnetic, vibrational, and optical properties	Free electron model, electrical conductivity and Ohm's law, 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.
Organic-inorganic materials	Phosphazene, borazines, TMDs: Synthesis, properties, bulk and nanostructures and important applications.
Materials for energy	Photovoltaic and photo-chemical effects, Exposure to material design for photovoltaic, LED/OLEDs, batteries, supercapacitors, and issues on energy conversions.
Introduction to different materials and relevant properties	Polymers, amorphous and quasicrystalline materials, alloys and compounds, nanomaterials

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, X-ray absorption spectra (XAS), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction). An introduction and applications to various chromatographic techniques will be discussed. **Molecular absorption** (ultraviolet-visible), luminescence, infrared, nuclear magnetic resonance, and mass spectrometry; electroanalytical methods (voltammetry); chromatographic separation (gas, high-performance liquid, and gas 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 spectroscopy	Atomic/molecular Absorption Instrumentation, Interferences in Atomic Absorption Spectroscopy, Atomic/molecular Absorption Analytical Techniques, Atomic/molecular Fluorescence Spectroscopy,
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). Advantages and disadvantages.
Introduction to Electroanalytical Methods	Types of Electroanalytical Methods: Conductometry, Electrogravimetry, Coulometry, Voltammetry Instruments for Measuring Cell Potentials, Voltammetry: Cyclic Voltammetry.

Chromatographic separations	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). Examples will be shared and discussed to which type of chromatography is applicable /appropriate for separation of compounds (trouble shooting).
Introduction to Thermal Methods of Analysis	Thermogravimetric Methods (TG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC).
Introduction and applications of electron microscopy (AS) and Atomic Force Microscopy	Introduction to and applications of transmission electron microscopy (TEM), scanning electron microscopy (SEM). An overview of the Atomic Force Microscopy Principle, modes of operation and applications.
Practicals (2 h)	1. Absorption and emission spectroscopic analysis of given commercial dyes to understand their nature of ground andexcited states. 2. HPLC separation of Benzoic acids and 4-Amino acetophenone and data analysis. 3. Estimation of methanol and toluene in Gas chromatography 4. MALDI mass analysis of macromolecules such as BSA protein. 5. TGA study for loss of moisture, drying, thermal stability of materials (organic and inorganic) ($CuSO_4.xH_2O$) (practicaland data analysis) (TR) 6. Study of crystallization (exothermic), melting (endothermic), glass transition of small organic molecule through DSC technique. 7. Bandgap analysis of Alq3 complex by suing UV-vis and Cyclic voltammetry. 8. Structure determination of given unknown organic samples by using NMR, UV-vis, IR, LC-MS techniques.

CHY652: Advanced Biochemistry (L : T : P = 3 : 0 : 0) (Elective Course)

The course is designed to elucidate biochemical reactions through the application of chemical knowledge. The progression of knowledge from chemistry will be cultivated to comprehend the functions of bio-macromolecules, including nucleic acids, proteins, carbohydrates, and lipids. Furthermore, the curriculum will cover the chemistry and biochemistry associated with these bio-macromolecules, illustrated with examples. The overarching goal is to understand the significance of the chemistry linked to biomolecules, encompassing carbohydrate metabolism, protein Sequencing, DNA Sequencing, DNA damage chemistry. The instructional approach will involve a combination of lectures, presentations, and assignments.

Course content

Carbohydrates	Carbohydrates metabolism; Kreb's Cycle and Glycolysis.
Peptide and protein Sequencing	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; Biological and chemical methods for DNA synthesis, DNA Sequencing; Sanger dideoxy method; Maxam Gilbert; Bisulfite methods. Reaction mechanism.
DNA replication & PCR	PCR, qPCR, RT-qPCR and applications in Forensics, Relationships, and medical Diagnosis
DNA chemistry	DNA damage; Methylation and deamination, depurination; Oxidative DNA damage; DNA-DNA crosslinks; DNA-Protein crosslinks; Mutagenesis; Diseases and carcinogenesis
Lipids and Vitamins	Fatty Acids, Classes of Lipids; Nomenclature of fatty acids; Examples of diff. Lipids; Phospholipids; Steroids, Lipid catabolism, β-Oxidation of Fatty Acids.
Hormones and Vitamins	Classifications of Hormones, Examples and Function of Hormones Classifications of Vitamins; Examples and Function of Vitamins
Enzymes	Co-factors, Co-enzymes, Apo-enzyme, Halo enzymes; Factors effecting Enzymes (Con., pH, T); Mechanism of Enzymes; Biosynthesis of cofactors; NAD+-NADPH; Biosynthesis of Niacin (Vitamin B3); FAD-FADH-FADH2; Thiamine pyrophosphate TPP.

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

In this course, students will be taught effective skills in presenting relevant literature, specifically, the most significant, landmarking, and the latest and relevant to their research areas of interest, utilizing reputable international journals. The focus is on developing proficiency in carefully analyzing and categorizing research publications. This process, done scientifically rigorously and personalized to each student's approach, will aid in developing their research interests. The faculty will critically evaluate presentations made by the students. The course will also cover skills such as preparing impactful slides, managing the allotted presentation time, and enhancing overall presentation capabilities. Furthermore, engaging in open discussions with students and faculty to gain an in-depth understanding of specific subjects will contribute to developing personality, initiating dialogue, and interacting confidently.