SHIV NADAR INSTITUTION OF EMINENCE DEEMED TO BE UNIVERSITY DELHI NCR | SCHOOL OF NATURAL SCIENCES

DEPARTMENT OF CHEMISTRY

School of Natural Sciences

About the Department:

Chemistry education at SNIoE provides a link between the fundamental principles governing the nature of the universe and the science of life, and spans traditional as well as a variety of inter-disciplinary areas. Chemistry, often referred as the central science, as it plays a vital role in nearly every other scientific field. At the undergraduate level, we offer B.Sc. (Research) in Chemistry. One can also combine a Minor in Chemistry with a Major in any other discipline at SNIoE and vice versa. University-wide elective courses in the curriculum allow students unprecedented freedom to explore subjects outside their chosen major; in some depth. This flexible and broad curriculum prepares students not just for a career in chemistry upon graduation, but for a leadership role in the world as well.

The Undergraduate Chemistry Experience

The chemistry curriculum at SNIoE provides both a broad background in chemical principles as well as in-depth study of chemistry or chemistry-related areas that build on this background. The chemistry curriculum is divided into three categories: introductory general chemistry, foundation courses providing breadth across sub-disciplines, and rigorous in-depth courses that build upon these foundations and develop critical thinking and problem-solving skills. Since chemistry is an experimental science, substantial laboratory work is an integral part of almost all our courses. The introductory general chemistry course provides a common grounding in basic chemical concepts for students with diverse backgrounds, develops basic mathematical and laboratory skills, and prepares students for the foundation courses. Foundation courses in general chemistry, analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry provide breadth and lay the groundwork for more in-depth course work.

Laboratory Experience

The chemistry laboratory experience at SNIoE includes synthesis of molecules; measurement of chemical properties, structures, and phenomena; hands-on experience with modern analytical instrumentation; and computational data analysis and modeling. All laboratory programs are conducted in a safe environment that includes adherence to national; and state regulations regarding hazardous waste management and laboratory safety including, facilities for chemical waste disposal, safety information and reference materials, and personal protective equipment available to all students and faculty. The chemistry laboratories at SNIoE are equipped with functioning fume hoods, safety showers, eyewashes, first aid kits, and fire extinguishers are readily available. Students are trained in modern chemical safety, to understand responsible disposal techniques, understand and comply with safety regulations, understand and use material safety data sheets (MSDS), recognize and minimize potential chemical and physical hazards in the laboratory, and know how to prevent and ability to handle laboratory emergencies effectively.

Problem-Solving Skills

As part of the SNIoE experience, students are expected to develop the ability to define problems, develop testable hypotheses, design and execute experiments, analyze data using statistical methods, and draw appropriate conclusions. The chemistry curriculum provides ample opportunities for developing both written and oral communication skills, as well as team skills. Our instructional programs incorporate team experiences in classroom and laboratory components of the chemistry curriculum.

Post-Graduate Programs

At the postgraduate level, SNIoE offers the following programs: Integrated B.Sc.-M.Sc. (Research), Integrated B.Sc.-M.Sc.-Ph.D., M.Sc. (Research), Integrated M.Sc.-Ph.D. and Ph.D. in chemistry. Foundation courses in the first semester ensure that all students, irrespective of the specialization, possess the requisite background to complete the course of study and benefit fully from the program. The integrated programs and the Ph.D. program in chemistry at SNU consists of a rigorous regimen of both broad-based and in-depth course work, development of project proposals, research and literature seminars, in-depth dissertation research under the supervision of a research advisor, and a public thesis defense.

Chemistry Careers

Chemistry offers good career opportunities for high quality graduates, in industry as well as in academia, in developed markets in India and abroad such as the US, Europe, Japan and Australia - the major employers being: industries related to agricultural technology, biotechnology, pharmaceuticals, and materials. IT industries working on artificial intelligence and related platforms do provide solutions to life sciences, biotechnology and health-care sectors; as well as R & D institutes and academia. Furthermore, chemists find job opportunities in various other sectors such as chemical industry, and advancement of career opportunities in forensic, food science and as health professionals.

Chemistry Research at SNIoE

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

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

- Bio-inorganic Chemistry
- Catalysis
- Chemical Biology
- Cheminformatics
- Computational Quantum Chemistry
- Chemical & Biology Crystallography
- Green Chemistry
- Materials Chemistry
- Medicinal Chemistry
- Metalloradical Chemistry
- Nano-Biotechnology
- Photoelectrochemistry
- Polymer Chemistry
- Protein Chemistry
- Supramolecular Chemistry

The specific research areas covered in the department can be found out from the departmental website:

(https://chemistry.snu.edu.in/research/areas-research).

Major in Chemistry

The basic undergraduate degree program offered by the Department of Chemistry is the Bachelor of Science: B.Sc. (Research) in Chemistry. In addition, Department of Chemistry is also offering specialization in Material Chemistry, Computational Chemistry and Chemical Biology in B.Sc. (Research) program (with Specialization).

Every chemistry undergraduate student of the University is required to take a number of credits from various courses as classified into the following categories:

- CCC (Common Core Curriculum courses offered by the university)
- UWE (University Wide Electives; courses so designated and offered by departments other than Chemistry)
- Introductory Chemistry courses (CHY100 – 199)
- Foundation Chemistry courses (CHY200 – 299)
- In-Depth Chemistry courses (CHY300 – 499)
- Electives/ Advanced Electives (CHY300 – 400 – 599)

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

- 110 = 73 credits in Core Chemistry Courses (Introductory + Foundation + In-Depth) + 13 PC(B)M/10 PCB credits (Physics/Life Sciences) + 12 PC(B)M/15 PCB credits (Chemistry electives) + 12 credits (Senior project)
- For 42 = 18 credits CCC courses + 18 credits UWE courses + 6 credits from either CCC and/or UWE/DSE (Department Selective Elective) category

Minor in Chemistry

Undergraduate students of the university who are not majoring in Chemistry have the option to take a Minor in Chemistry.

Academic Requirements for Chemistry Minor:

27 credits = 24 credits in compulsory courses [12 Introductory (Category A) + 12 Foundation (Category B)] + 3 credits of Chemistry In-Depth/Elective courses (Category C).

Category	Course	Course Title	L:T:P	Credits
				Minor
A	CHY111	Chemical Principles	3:1:1	12
	CHY211	Chemical Equilibrium	3:0:1	
	CHY214	Physical Methods in Chemistry	2:0:1	
B	CHY122	Basic Organic Chemistry-I	2:1:1	12
	CHY144	Inorganic Chemistry-I	3:0:1	
	CHY221	Basic Organic Chemistry-II	2:1:1	
	CHY222	Chemistry of Carbonyl Compounds	3:0:1	
	CHY242	Coordination Chemistry	3:0:1	
	CHY245	Inorganic Chemistry-II	2:1:1	

	CHY311	Chemical Binding	3:1:0	
	CHY313	Molecular Spectroscopy	3:1:0	
A course from "category B" cannot count towards both Major and Minor requirements. For example, Biotechnology students cannot count CHY122 towards the Minor degree as it is a compulsory course in their Major.				
C	CHYXYZ	Any course from Chemistry course catalogue	3:0:0	3
		Credits		**27**

Chemistry Course Catalogue:

The chemistry program at SNIoE provides both a broad background in chemical principles and in-depth study of chemistry or chemistry-related areas that build on this background. The chemistry curriculum is divided into three parts: (1) the introductory chemistry experience, (2) foundation course work that provides breadth, and (3) rigorous in-depth course work that builds on the foundation. Because chemistry is an experimental science, substantial laboratory work is an integral part of this experience.

Introductory or General Chemistry

The introductory or general chemistry experience plays a vital role in educating all students. The introductory courses provide a common background for students with a wide range of high school experiences, and allow a period for consolidation of chemical concepts, as well as mathematical and laboratory skills. For students pursuing a chemistry major, the introductory chemistry courses provide preparation for the foundation course work, ensuring that students know basic chemical concepts such as stoichiometry, states of matter, atomic structure, molecular structure and bonding, thermodynamics, equilibria, and kinetics. Students also need to be competent in basic laboratory skills such as safe practices, keeping a notebook, use of electronic balances and volumetric glassware, preparation of solutions, chemical measurements using pH etc.

❖ **CHY103: Mathematics for Chemistry-I** (4 credits: 3 Lectures + 1 Tutorial + 0 Lab) Monsoon

This course will introduce the students to various basic mathematical methods for chemists. The methods involve the basics of calculus, vectors and matrices, first and second-order differential equations and their solution, series, and complex numbers. The course will have lectures and tutorial classes with several practice sessions. On successful completion of the course, students will have:

(a) Sufficient knowledge of mathematics needed for Chemistry.

(b) Understanding of the mathematical concepts necessary for Physical science as well.

(c) Develop capability to solve numerical problems related to physical chemistry and basic physics.

Course Content

Functions of a Single Variable (Differentiation): Functions, Continuity, Differentiation, Maxima, and minima.

Functions of a Single Variable (Integration): Definition of an integral, Methods of Integration, Improper integrals.

Functions of Several Variables: Partial derivatives, Total differentials, Chain rules for partial differentiation, Maxima and minima, Multiple integrals.

Ordinary Differential Equations: Linear first-order differential equations, Homogeneous linear differential equations with constant coefficients.

Vectors: Representation of vectors, Products of vectors, Basic vector calculus.

Plane Polar Coordinates and Spherical Coordinates: Plane polar coordinates, Spherical coordinates

Series and Limits: Power Series, Taylor series, Maclaurin Series.

Complex Numbers: Complex numbers and the complex plane, Euler's Formula and the polar form of complex numbers.

Determinants: Definition of a determinant, Properties of determinants.

Matrices: Matrix algebra, Inverse of a matrix, Orthogonal matrices.

Prerequisites: None

❖ **CHY104: Mathematics for Chemistry-II** (4 credits: 2 Lectures + 2 Tutorial + 0 Lab) Spring

This course will introduce the students to various basic mathematical methods for chemists. The methods involve some advanced concepts of calculus, numerical methods, probability and statistical methods, polynomials etc. Students in 1st and 2nd year B Sc (Research) in Chemistry are encouraged to take this course. Course will have lectures and tutorial classes with several practice sessions.

Course Content

Functions of Several Variables: Recap of Partial derivatives, Total differentials, Chain rules for partial differentiation, Euler's theorem, Maxima and minima, Multiple integrals, The Dirac Delta Function.

Series and Limits: Convergence and divergence of infinite series, Power Series, Maclaurin Series, Complex Fourier Series, Fourier Transforms (Fourier Integrals).

Power Series Solutions of Differential Equations: Oscillatory solutions, The power series method, Series solutions of Legendre's equation.

Orthogonal Polynomials: Legendre Polynomials, Orthogonal Polynomials.

Matrices: Unitary matrices, Matrix eigenvalue problems and Diagonalization of matrix.

Vector Spaces: The axioms of a vector space, Linear independence, Inner product spaces, Complex inner product spaces.

Probability: Discrete distributions, The multinomial distribution, Continuous distributions, Joint probability distributions, Probability distributions in quantum mechanics, Time average.

Statistics (Regression and Correlation): The Combination of Errors, Linear regression analysis, Correlation analysis, Error propagation of measurements.

Numerical Methods: Roots of equations, Numerical integration, Summing series, Systems of linear algebraic equations.

Prerequisites: Mathematics for Chemists-I (CHY103)

❖ **CHY111: Chemical Principles** (5 credits: 4 Lectures/Tutorial + 3-hour Lab) Monsoon

This course will focus on introductory chemical principles, including periodicity, chemical bonding, atomic and molecular structure, equilibrium and principles of various analytical techniques. Students will explore stoichiometric relationships in solution and gas systems, which are the basis for quantifying the results of chemical reactions. Understanding chemical reactivity leads directly into discussion of equilibrium and thermodynamics, two of the most important ideas in chemistry. Equilibrium, especially acid/base applications, explores the extent of reactions while thermodynamics helps understanding if a reaction will happen. The fundamentals of organic chemistry will be discussed that includes origin of organic compounds, functional groups, substitution and elimination reaction and basics of stereochemistry and name reactions.

Course Content

Unit-1: Atomic structure, Periodic table, VSEPR, Molecular Orbital Theory and Spectroscopy:

a) Introduction atomic structure, concept of atom, molecules, Rutherford's atomic model, Bohr's model of an atom, wave model, classical and quantum mechanics, wave particle duality of electrons, Heisenberg's uncertainty principle, Quantum-Mechanical model of atom, The Bohr's theory of the hydrogen atom and spectra.

b) Concept of Atomic Orbitals, representation of electrons move in three-dimensional space, wave function (Ψ), Radial and angular part of wave function, radial and angular nodes, Shape of orbitals, the principal (n), angular (l), and magnetic (m) quantum numbers, Pauli exclusion principle.

c) Orbital Angular Momentum (l), Spin Angular Momentum (s), HUND's Rule, The *aufbau* principle.

d) Shielding Effect, Effective Nuclear Charge, Slater's rule

e) Periodic properties elements

f) Lewis structures

g) Valence shell electron pair repulsion (VSEPR)

h) Valence-Bond theory (VB), Orbital Overlap, Hybridization, Molecular Orbital Theory (MO) of homo-nuclear diatomic molecules.

i) Molecular Orbital Theory of hetero-nuclear diatomic molecules.

j) Spectroscopy: Basic of atomic and molecular spectroscopy, regions of the spectrum: Radiofrequency (NMR/EPR, change of spin), Microwave (rotational Spectra), Infra-red (vibrational spectra), UV-Vis (electronic spectra)

k) Bond energies of various single and double bond and their vibrational frequency values in IR. Vibrational Spectroscopy of simple Harmonic oscillators like H_2, O_2, N_2, HCl, CO, NO, and CO_2, degree of freedom, stretching and bending.

l) IR spectra of different functional groups such as -OH, -NH_2, -CO_2H etc.

m) UV-Vis Spectroscopy of organic molecules, Electronic Transitions, Beer-Lambert Law, Chromophores.

Unit-2: The Principles of Chemical Equilibrium and Kinetics:

a) **Thermodynamic System & Surroundings:** Introduction

b) **Laws of Thermodynamics:** Zeroth Law, First Law (Heat & Work; State and Path Functions; Different Thermodynamic Processes; Thermal Process using an ideal gas; Specific Heat capacities; Enthalpy; Thermochemistry (Hess's law)), Second Law: Entropy (Heat Engines; Carnot's Principle and the Carnot Engine; Refrigerators and Air Conditioners), Third Law (Variation of Entropy with Temperature, Pressure and Volume; Absolute Entropy; Standard Molar Entropy; Calculation of Entropy; Probability and Entropy), Energy (Gibbs and Helmholtz; Maxwell Relations).

c) **Phase Equilibrium:** Phase Diagram; Gibbs Phase Rule; Degrees of Freedom; Phases.

d) **Chemical Equilibrium:** Equilibrium Law.

e) **Chemical Kinetics:** Rate of a reaction, rate law and specific rate constant, integrated rate equations and half-life (zero, first and second order reactions), Time constant, Activation energy, Arrhenius equation.

f) **Catalysis:** Homogeneous and Heterogeneous - Basics, Characteristics and Features.

Unit-3: Organic Chemistry:

a) **Introduction to organic chemistry:** Examples of various organic chemicals of natural and industrial importance, Bulk vs fine chemicals

b) **Functional group:** Types and nature

c) **Physical properties of organic compounds:** A general view on physical properties of organic compounds with variation of functional groups: melting point and boiling point, solubility, acidity and basicity, dipole moment, colour (resonance, phenolphthalein, nature pigments), alkanes vs polyethylene, fun facts (proteins, natural acid, fats)

d) **Substitution reactions:** S_N1 and S_N2

e) **Elimination reactions:** Hoffmann and Saytzeff elimination

f) **Name reactions:** Markownikoff and Anti-Markownikoff reaction (ionic *vs*. free radical addition)

g) **Stereochemistry:** definition, classification in isomerism

h) **Compounds containing single bonds:** conformational and configurational isomerism. Isomerism in (ethane, butane and cyclohexane for mono and di-substituted)

i) **Chirality:** Concept of chirality (up to two carbon atoms), chiral, achiral, optical isomerism, enantiomers and diastereomers, R and S nomenclature with C.I.P rules, optical activity, rotation, racemic mixture

j) **Compounds containing double bonds:** Geometrical isomerism: cis–trans, Z and E, notations with C.I.P rules.

Lab Schedule:

Exp. No.	Experiment Name
1	Introduction to lab/ Grading scheme/Safety Rules
2	Safety Quiz - Displaying Data Graphically
3	**Expt.1-** Sugar Content of Common Drinks
4	**Expt.2-** Stoichiometry of H_2O_2 decomposition
5	**Expt.3-** Determination of Conc. of an Unknown coloured soln.
6	**Expt.4-** Total Hardness of Water
7	**Expt.5-** Synthesis of Nylon
	Make-up-week
8	**Expt.6-** Recycling Aluminium foil / Technique Grade
9	**Expt.7-** Analysis of Common Functional Groups
10	**Expt.8-** Synthesis of aspirin / Technique Grade
11	**Expt.9-** Analysis of aspirin
12	Make-up-week

Prerequisite: None.

❖ **CHY114: Molecular Modelling** (2 credits: 1 Lectures + 2 hour Lab) Spring

The importance of spatial visualization and model thinking in chemistry cannot be overemphasized. This course aims to provide students with a working understanding of the use of computers in modern chemistry practice, and enable them to develop their skills in visualizing molecular models. It will also introduce students to the Linux operating system, and for those without prior programming experience, introduce them to algorithmic thinking and help them develop programming skills.

Course Content

Computational tools for Molecular Modelling: The Linux Operating system, Useful Commands, Linux Shell and Shell Scripting, Useful Hardware and Software for Molecular Modelling

Concepts in Molecular Modelling: Chemical Drawing (Chemical Drawing with ChemDraw, Three Dimensional Effects in Chemical Structures, Representation of Optical isomerism)

Molecular Structure Databases [Cambridge structural Database (CSD), Protein Data Bank(PDB), File format and information in PDB and CSD databases]

Molecular Modelling (Molecular Graphics, 3-D Models of Organics and Biomolecules, Coordinate systems, Potential Energy Surfaces

Case Study: Visualization of 3D Models with Gauss View/Avogadro/Chemcraft

Introduction to Perl (Data types, Arrays and lists, Control structures, Regular expressions, Input/output and file handling)

Empirical Force Field Models (Molecular Mechanics): Balls on Springs (Vibrational Motion, Force law, a simple Diatomic Molecule, Morse Potential

Force Fields (Bonded Terms in Force Field, Non-bonded Terms, Effective Pair Potential, Hydrogen Bonding in Molecular Mechanics

Applications of Molecular Mechanics: Force-field parameterization for Biological systems, Inorganic molecules and Solid state systems, Solvent Modelling in Molecular mechanism, Calculating Thermodynamics Properties using Molecular Mechanics, Energy Minimisation and Exploring Energy Surface

Case Study: Force-Field Parametrization of simple Organic Molecules

Computer Simulation and Structure-based De Novo Ligand Design: Introduction, Calculations of simple Thermodynamical Properties, Molecular Dynamics Simulations (Molecular Dynamics Using Simple Models, Constraint Dynamics, Conformational Changes from Molecular Dynamics Simulations)

Analysing the Results of the Simulations and Estimating errors: Molecular Docking (Introduction, Scoring Functions, Applications of Docking

Case Study: Setting up a Molecular Dynamics Simulation of Insulin in water as a Solvent

Prerequisites: None.

- **CHY122: Basic Organic Chemistry I** (4 credits: 2 Lectures+ 1 Tutorial + 3 hour Lab) Spring

The course is designed to assist a swift transition of the knowledge acquired by students during school level to university level. The further advancement of in-depth knowledge in organic chemistry subject is designed via a stepwise procession from basic introductory level to advance level in subsequent years. The course covers the fundamental aspects of the basic organic chemistry principles via structure analysis approach. Students are required to complete all the assignments individually with a critical thinking. Practicals are designed to provide further insight on theoretical knowledge.

This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

Course Content

Intermolecular forces of attraction: van der Waals forces, ion-dipole, dipole-dipole and hydrogen bonding, Homolytic and heterolytic bond fission. Hybridization- Bonding, Electron displacements: Inductive, electromeric, resonance, hyperconjugation effect, Reaction intermediate- their shape and stability: carbocations, carbanions, free radicals, carbenes, benzyne, Acidity and basicity of organic molecules: Alkanes/Alkenes, Alcohols/Phenols/Carboxylic acids, Amines pKa, pKb. Electrophiles and nucleophiles. Nucleophilicity and Basicity, Aromaticity and Tautomerism, Molecular chirality and Isomerism: Cycloalkanes (C3 to C8) Relative stability, Baeyer strain theory and Sachse Mohr theory, conformations and conformational analysis: Ethane, n-butane, ethane derivatives, cyclohexane, monosubstituted and disubstituted cyclohexanes and their relative stabilities. Stereochemistry (Structural- and Stereo-isomerism), Molecular representations: Newman, Sawhorse, Wedge & Dash, Fischer projections and their inter conversions, Geometrical isomerism in unsaturated and cyclic systems: cis–trans and, syn-anti isomerism, E/Z notations. Geometrical isomerism in dienes- Isolated and conjugated systems, determination of configurations, Chirality and optical isomerism: Configurational isomers. Molecules with one or two chiral centres- constitutionally symmetrical and unsymmetrical molecules; Enantiomers and diastereomers. Optical activity, disymmetry, meso compounds, racemic modifications and methods of their resolution; stereochemical nomenclature: erythro/threo, D/L and R/S nomenclature in acyclic systems. Measurement of optical activity: specific rotation.

Lab Schedule:

S. No	Experiments
1	Introduction to lab/ grading scheme/safety Rules
2	**Expt.1**- Intermolecular forces
3	**Expt.2**- Calibration of a thermometer & - Melting point and boiling point determination of unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
4	**Expt.3-** Acidity and basicity: pHmetry using a Vernier probe vs volumetric titration
5	**Expt.4-** Separation of an acidic and a neutral substance by extraction in microscale
6	**Expt.5 -** Separation of an acidic, a basic and a neutral substance by extraction in macroscale
7	**Make-up-week**
8	**Expt.6 -** Paper chromatography for separation of amino acids
10	**Expt.7 -** Thin layer and column chromatography.
12	**Expt.8 -** Synthesis and characterization: recrystallization (Schötten Baumann reaction)
13	**Expt.9 -** To find the optical rotation of a chiral molecules
14	**Expt.10 -** NMR experiment
15	**Make-up-week**

Prerequisite: Chemical Principles (CHY111).

❖ **CHY144: Inorganic Chemistry-I** (3 credits: 2 Lectures + 0 Tutorial + 1 Lab) Spring

This course aims at helping the student to understand the concept of chemical bonding and acid-base.

Course Content

Chemical bonding: Molecular structure and bonding: Fazan's Rule, VSEPR, BENT's rule, Involvement of d orbital in hybridization, How VSEPR theory is different from hybridization concept, Valence bond theory - homonuclear diatomic molecules - polyatomic molecules, Molecular orbital theory of heteronuclear diatomic molecules (CO, NO, HF etc.), bond properties, polyatomic molecules, concept of HOMO, LUMO and SOMO; Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids. Weak Chemical Forces: Hydrogen bonding (theories of hydrogen bonding, valence bond treatment), receptor-guest interactions, Halogen bonds. Effects of chemical force, melting and boiling points, Inert-pair effect, Borane chemistry (Structure and bonding), Bonding of noble gas compounds, Defects in solids. Stoichiometric defect: Schottky and Frenkel defects, Non-stoichiometric imbalance in crystals (outline). Crown ether complexes of alkali metals.

Acid-Base: Introduction, Theories of acids-bases: Arrhenius theory, Bronsted-Lowry theory, Conjugate Acid-Base pairs, Solvent system definition, Lux concept, Lewis theory, Properties of Lewis Acids and Bases, Complex formation in acid-base reaction, Gas-phase proton affinity, acids and bases in water, levelling effect, general strength of acid and base; the concept of Hard and Soft Acids and Bases (HSAB), Magic Acids/Superacids.

General principle of equilibrium, equilibrium in solutions of acids and bases: strong acids and strong bases, weak acids and weak bases, polyprotic acids and bases, the equilibrium constant, Strength of acids and bases in aqueous solution in terms of K_a, K_b; the pH scale, pK_w, pK_a, pK_b, etc. (numerical problems).

Aqueous solutions of salts, hydrolysis of salts, equilibrium in hydrolysis of salts: salts derives from weak acids and strong bases, salts derives from strong acids and weak bases, salts derives from weak acids and weak bases, numerical problems on hydrolysis of salts.

Buffer solutions: pH of a buffer solution, Henderson equations (numerical problems).

Acid-base titrations: choice of indicator, neutralization of a strong acid by a strong base, neutralization of a weak acid with a strong base, neutralization of a weak base with a strong acid, neutralization of a weak acid by a weak base, neutralization of a weak acid with a strong base - neutralization of a weak base with a strong acid - neutralization of polyprotic acids with strong base.

Solid–Solution Equilibrium: Solubility and solubility product (K_{sp}), common ion effect, effect of H^+/OH^- and complexing agents. Application of the concept in qualitative analysis; calculation on pH condition and precipitation.

Oxidation and Reduction: redox equilibrium and ion–electron method of balancing redox equations, disproportionation relations. Chemistry in Non-aqueous solvents (Common non-aqueous solvents, the solvent concept, coordination model, chemistry in liquid NH_3, liquid HF, $SOCl_2$, liquid H_2SO_4, fluorosulfonic acids, N_2O_4, and SO_2).

Lab Schedule:

S. No	Experiments

1	**Expt.1-** Analysis of mixture of carbonate and bicarbonate
2	**Expt.2-** Permanganometry (Fe^{2+} and Fe^{3+} mixture)
3	**Expt.3-** Dichromatometry (Fe^{2+} and Fe^{3+} mixture, role of indicator)
4	**Expt.4-** Determination of pKa values of acetic acid and oxalic acid
5	**Make-up-week**
6	**Expt.5-** Determination of solubility product
7	**Expt.6-** Partition coefficient of iodine between two immiscible solvents
8	**Expt.7-** Determination of inorganic radicals by flame test, spot test and UV-Vis study in a mixture
9	**Expt.8-** Determination of concentration of $CuSO_4$ in a solution by UV-Vis
10	**Make-up-week**

Prerequisite: Chemical Principles (CHY111).

Foundation Courses

Foundation courses provides breadth and lays the groundwork for the in-depth course work in each of the five major areas of chemistry: analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry. The chemistry laboratory experience at SNU includes synthesis of molecules; measurement of chemical properties, structures, and phenomena. Students get hands-on experience with modern instrumentation on a variety of analytical instruments, including spectrometers, and are expected to understand the operation and theory of modern instruments and use them to solve chemical problems as part of their laboratory experience.

- **CHY211: Chemical Equilibrium** (5 credits: 3 Lectures + 1 Tutorial + 3 hour Lab) Monsoon

This course is deigned to understand thermodynamic principles already familiar to students from earlier courses. The course will culminate with an introduction to statistical thermodynamic and molecular reaction dynamics. The course content will be exemplified using various real examples/case studies.

Course Content

Kinetic Theory of Gases: Introduction of Kinetic Theory of Gases, Maxwell-Boltzmann Distribution of Velocities and energy, Effect of Temperature on Energy distribution.

Phase Equilibria: Phase diagrams and impact on material sciences, Phase transitions, Chemical equilibrium and its impact on technology and biochemistry, Changes in equilibria with temperature and pressure.

Colligative properties: Raoult's Law, Ideal and non-ideal mixtures.

Chemical Kinetics: Determination of rate, order and rate laws, Impact of Chemical Kinetics on Biochemistry, Theories of Reaction rates; Collison theory, thermodynamics theory, statistical theory, transition state theory-its application and formulation.

Catalysis: Homogenous and Heterogenous Catalysis, General Catalytic Mechanisms; Arrhenius Intermediate, van't Hoff Intermediates, Activation energies, Acid-Base Catalysis; Mechanism, Catalytic Activity, Salt effects, Enzyme Catalysis; Effect of Substrate, effect of pH, effect of temperature, Enzyme Mechanism.

Chemistry of Solutions and Surfaces: Osmosis and reverse osmosis; Osmotic Pressure and effect of Vapour pressure lowering, Adsorption and Chromatography, Effect of temperature and pressure, Langmuir Isotherm, Gibbs Adsorption Isotherm, Ion Exchange columns and water purification.

Lab Schedule:

S. No	Experiments
1	Safety rules/quiz; Download Vernier 3.8 for next week
2	**Expt.1-** Determine K_{eq} for (KSCN) + $Fe(NO_3)_3$
3	**Expt.2-** Determination of Enthalpy (Bleach-Acetone)
4	**Expt.3-** Determination of equilibrium constant for Bromocresol Green
5	**Expt.4-** Acid Rain experiment
	Make up week
6	**Expt.5-** Arrhenius equation using $KMnO_4$ – Oxalic Acid
9	**Expt.8-** Order of reaction with respect to Crystal Violet (Crystal Violet-OH^-)
10	**Expt.9-** Order of reaction with respect to OH^- (Crystal Violet- OH^-)
11	**Expt.10-** Crystal Violet-OH^- (Arrhenius)
	Make up week
	VIVA

Prerequisites: Chemical Principles (CHY111).

❖ **CHY212: Chemical Applications of Group Theory** (3 credits: 3 Lectures) Monsoon

This course deals with a systematic mathematical analysis of symmetry in chemical systems using group theory. Group theory provides considerable insight into the chemical and physical properties of molecules once its symmetry has been classified. We can determine whether a spectroscopic transition is allowed or forbidden by using selection rules associated with symmetries, and we can interpret the bands in the Infrared and Raman spectra. Moreover, if the symmetry of the molecular orbital wave function is known, we can learn information about bonding. Some simple applications of group theory in chemistry will be covered in this course.

Course Content

Principles of group theory: Importance of symmetry and group theory in chemistry, Symmetry elements and symmetry operations, associated symmetry operations, Definition and properties of group, similarity transformation, class of a group, Point group: molecular point groups (symmetry classification of molecules), Product of symmetry operations, group multiplication tables, Matrix representation of symmetry operations, Matrix representation of point groups, character representation of point group, Reducible representation and irreducible representation of point group, Great Orthogonality Theorem, character table.

Application of group theory in chemistry: Projection operator, symmetry adapted linear combinations (SALC), Molecular orbital for sigma bonding, Molecular orbitals for pi bonding, Direct product representation, Basics of infrared and Raman spectroscopy, Infrared and Raman active modes of molecular vibrations, Mutual exclusion principle, some illustrative examples, Basics of electronic spectroscopy, Selection rules of spectroscopic transitions.

Prerequisites: Chemical Principles (CHY111); Mathematics for Chemists-I (CHY103)/(MAT103).

❖ **CHY214: Physical Methods in Chemistry** (3 credits: 2 Lectures + 0 Tutorial + 2 hour Lab) Monsoon

Analyses of compounds are an integral aspect of chemistry. We get to know the structure, spatial orientation and purity of compounds we synthesize through analysis, which helps us to advance in our investigation. To address this purpose a bevy of instruments ranging from UV spectroscopy, IR spectroscopy to High Pressure Liquid Chromatography are available. However accurately understanding the output from these instruments is an essential attribute for a successful chemist. The purpose of this course is to familiarize the students with the basic principles of spectroscopic and diffraction methods that are instrumental to the analysis of molecules and structures in the day-to-day life of a chemist. In this course, we will learn to interpret and understand working of various types of analytical instruments commonly used for analysis in a chemistry lab.

Course Content

Unit-1: UV-Visible spectroscopy, **Fluorescence Spectroscopy**, **Nuclear Magnetic Resonance (NMR) spectroscopy, Mass spectrometry, Data Analysis**

A. **UV-Visible spectroscopy**: Concept of absorption spectroscopy, atomic vs molecular absorptions, concept of color, effect of conjugation. Bathochromic, hypsochromic, hyperchromic and hypochromic shifts.

B. **Fluorescence Spectroscopy**: Principles of fluorescence, Jablonski Diagram, solvatochromism, Stoke's shift, Quantum yield, parameters affecting photophysical property.

C. **Nuclear Magnetic Resonance (NMR) spectroscopy**: Spinning nucleus, effect of an external magnetic field, precessional motion and precessional frequency, precessional frequency and the field strength, proton NMR spectrum, solvents used in NMR, solvent shift and concentration effect and hydrogen bonding, deuterium exchange.

D. **Mass spectrometry**: Introduction to mass spectroscopy: isotope effect, fragmentation patterns. McLafferty rearrangements, chemical ionization.

E. **Data Analysis**: Uncertainties, errors, mean, standard deviation, least square fit.

Unit-2: Microwave and Vibrational spectroscopy, Chromatography

F. **Microwave or Rotational Spectroscopy:** Principal axes of rotation and three principal moments of inertia, Classification of molecules based on moments of inertia, Rigid (diatomic) rotator model, Rotational energy levels and rotational selection rule and transitions, Rotational spectra of carbon monoxide and water vapor, Basic instrumentation of rotational spectroscopy.

G. **Infra-Red spectroscopy**: Molecular vibrations, Modes of vibration, Factors influencing vibrational frequencies: coupling of vibrational frequencies, hydrogen bonding, electronic effects, The Fourier Transform Infrared Spectrometer, Calibration of the Frequency Scale, Absorbance and Transmittance scale, intensity and position of IR bands, fingerprint region, and interpretation of IR spectra of simple organic molecules, basic mention of Raman Spectroscopy including the mutual exclusion principle, Raman and IR active modes of CO_2.

H. **Chromatography:** Principle of chromatography, Thin Layer chromatography (TLC), High-Performance Liquid Chromatography (HPLC), Liquid chromatography-Mass Spectrometry (LC-MC), Application of chromatography.

Unit-3: Single-crystal X-ray Diffraction (Small molecules & Macromolecules) & Thermal Characterization:

I. **X-ray Diffraction**: X-ray generation, Classification and Sources; Diffraction of X-rays, Bragg's Law; Lattice, Planes and Miller indices; Introduction on Point group and space group; Crystal growth (small molecules & proteins); Selection of Single-crystals; Data collection strategy; Overview of data analysis and preliminary structure determination.

J. **Thermal characterization**: Differential scanning calorimetry (DSC) and Thermo Gravimetric Analysis (TGA).

Lab Schedule:

S. No	Experiments
	Unit-1
1	**Expt.1-** Introduction to UV-Vis/photoluminescence/NMR and Grading scheme/Safety Rules
2	**Expt.2-** Characterization of various solvents by UV-Vis technique - Displaying Data Graphically
3	**Expt.3-** Characterization of various organic dyes by UV-Vis technique- Displaying Data Graphically
4	**Expt.4-** Characterization of various organic luminescence dyes by photoluminescence spectrometer- Displaying Data Graphically
5	**Expt.5-** Characterization of various organic molecules by NMR technique- Displaying Data Graphically
6	**Expt.6-** Determination of molecular mass of organic compounds
	Unit-2
7	**Expt.7- I**R: Determination of Functional Groups
8	**Expt.8-** IR: Determination of Functional Groups
9	**Expt.9-** Identification of stretching, bending and combination bands of water
10	**Expt.10-** Study of isotope effect using IR spectroscopy
11	**Expt.11-** TLC/HPLC Experiment: Working principle and demonstration
12	**Expt.12-** TLC/HPLC Experiment: Separation of small molecules
	Unit-3
13	**Expt.13-** Sample preparation and crystallization (Small molecule)
14	**Expt.14-** Small molecule crystal selection, data collection
15	**Expt.15-** Small molecule structure determination
16	**Expt.16-** Sample preparation and Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA) experiments (small molecule)
17	**Expt.16-** DSC and TGA data analyses and interpretations

Prerequisites: Chemical Principles (CHY111).

❖ **CHY221: Basic Organic Chemistry-II** (4 credits: 2 Lectures + 1 Tutorial + 3-hour Lab) Monsoon

Answer to the question, “Why the reaction proceeds via one mechanism despite so many pathways are possible?” will be provided. The course will assist to utilise the nomenclature, structures, functionalities, properties of organic structures to determine probable reaction mechanisms. Assignments are designed in such a way to illustrate their problem solving skills using basics of organic chemistry with a critical thinking. Practicals are designed to allow a good coverage and hands on experience on basic lab skills synthesis and purification. There will be continuous practice sessions during the class hours.

Course Content

Organic reactions; nucleophilic substitution, elimination, addition and electrophilic aromatic substitution reactions with examples will be studied. A brief description on methods of preparation of alkyl halides will be provided followed by

Substitution reactions: Nucleophilic substitution vs. elimination. Free radical halogenation, relative reactivity and selectivity principle, Allylic and benzylic bromination, Nucleophilic Subsititution (S_N1, S_N2, S_N1', S_N2', S_Ni) mechanisms with stereochemical aspects and effect of solvent etc., examples. Bredt's rule, Electrophilic aromatic substitution will be studied in detail, Electrophilic Substitution (S_NAr, Addition Elimination vs. Elimination addition) (including preparation from diazonium salts). Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Elimination reactions: Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cB reactions, Saytzeff and Hofmann eliminations

Addition reactions: To begin with, chemistry of Alkanes sigma bonds will be atught, Chemistry of alkanes: Formation of alkanes, Organometallic reagents, Wurtz reaction, Wurtz-Fittig reactions, their utilty.

Alkenes and alkynes pi bonds: Electrophilic additions their mechanisms (Markownikoff/ Anti-Markownikoff addition), Mechanism of oxymercuration-demercuration, hydroboration oxidation, ozonolysis, reduction, 1,2-and **Addition reactions:** 1,4-addition reactions in conjugated dienes and Diels-Alder reaction; electrophilic and nucleophilic additions. Hydration to form carbonyl compounds, alkylation of terminal alkynes.

Lab Schedule:

S. No.	Experiments
1	Introduction to the lab notebook requirements and grading
2	**Expt.1-** Separation of two compounds, purification by recrystallization, Thin Layer Chromatography, Column Chromatography.
3	**Expt.2-** Nucleophilic substitution bimolecular reaction (S_N^2).
4	**Expt.3-** Nucleophilic substitution unimolecular reaction (S_N^1).
5	**Expt.4-** Oxidation of benzaldehyde to benzoic acid.
6	**Expt.5-** Borohydride reduction of a ketone: hydrobenzoin from benzil.
7	**Make up week/VIVA**
8	**Expt.6-** Benzoylation of a given compound
9	**Expt.7-** Halogenation of acetanilide/benzanilide
10	**Expt.8-** Bromination of stilbene
11	**Expt.9-** Synthesis of dye. Recording UV-Vis in different media.
12	**Expt.10-** Alkylation of saccharin with iodoethane
13	**Make up week/VIVA**

Prerequisites: Basic Organic Chemistry-I (CHY122).

❖ **CHY222: Chemistry of Carbonyl Compounds** (4 credits: 2 Lectures + 1 Tutorial + 3 hour Lab) Spring

Structure and bonding in carbonyl groups, reactivity, nucleophilic addition and substitution reactions at the carbonyl centre, α-anion chemistry, chemistry of active methylene compounds and redox reactions involving carbonyl groups are covered in this course.

Course Content

- **Introduction to carbonyl compounds:** structure and bonding in carbonyl compounds, acidity and basicity-pKa of carbonyls, tautomerism in carbonyl compounds - the keto-enol equilibrium, reactivity of carbonyl group, how to write reaction mechanism

- **Nucleophilic-electrophilic reactivity of carbonyl compounds:** chemistry of enols and enolates, addition–dehydration (Aldol reaction); ester condensation (Claisen reaction), fragmentation of β-dicarbonyls, alkylation of enolates
- **Nucleophilic substitutions on the carbonyl group-The carboxylic acid family:** reactivity of carboxylic acid family**,** esters and thioesters- synthesis, structure and reactivity**,** amides- synthesis, structure and reactivity**,** acyl halides and anhydrides- synthesis, structure and reactivity**,** organometallic reagents-Grignard reaction & and alkyl lithium**,** enantiomeric resolution
- **Oxidation-reduction reactions of carbonyl compounds:** Enantiomeric resolution, oxidation of carbonyls - Jones oxidation, Oppenauer oxidation, functional group interconversion through oxidation**;** reduction of carbonyls: $NaBH_4$/$LiAlH_4$/diborane reduction, Cannizaro reaction, MPV reduction, Clemmensen reduction, Wolff-Kishner reaction, Rosenmund reduction, DIBAL reduction, reduction of acids, amines and nitriles.
- **Nucleophilic additions to carbonyl groups:** Cyanohydrin formation**,** acetals, ketals and hydrates**,** Grignard reaction, reaction with alkyl lithium**,** reactions with nitrogen nucleophiles-imine and hydrazine formation**,** nucleophilic addition to carbonyl analogues-cyanides, imines etc.

Lab Schedule:

S. No.	Experiments
1	Introduction to the lab notebook requirements and grading
2	**Expt.1-** Osazone reaction: Identification of an unknown Sugar (addition reaction)
3	**Expt.2-** Preparation of Dibenzylideneacetone (Aldol condensation)
4	**Expt.3-** Synthesis of Isopentyl acetate (Esterification)
5	**Expt.4-** Benzilic acid from Benzil (Rearrangement reaction)
6	**Expt.5-** Synthesis of the Commercial Antidepressant Moclobemide (Amide bond formation)
7	**Make up week/VIVA**
8	**Expt.6-** Preparation of Benzopinacol from benzophenone (Reduction by Zn metal)
9	**Expt.7a-** Preparation of Benzyl alcohol from Benzaldehyde (Cannizzaro Reaction)
10	**Expt.7b-** Preparation of Benzoic acid from Benzaldehyde (Cannizzaro Reaction)
11	**Expt.8-** Estimation of Vitamin C (Iodometric method)
12	**Make up week/VIVA**

Prerequisites: Basic Organic Chemistry-I (CHY122) and Basic Organic Chemistry-II (CHY221).

❖ **CHY 241: Electrochemistry** (2 credits: 2 Lectures) Monsoon

This course aims at helping the student to understand the basic of electrochemistry. The course covers the fundamentals of electrochemistry.

Course content

Introduction: General discussion about oxidation and reduction, electron transfer vs atom transfer, oxidation no, concept of electrochemistry,

Electrochemical cell: Electrodes, salt bridge and its function etc. battery; types of cell: electrolytic cell *vs*. galvanic cell; concentration cell vs chemical cell, How to construct a voltaic cell?

Definition: Electrode potential, Std. potential and Formal potential; Physical significance of electrode potential.

Types of electrodes: (i) metal electrode, advantage of amalgam electrode; (ii) non-metal electrode, e.g. hydrogen gas electrode, glassy carbon electrode.

Electroanalytical techniques: Potentiometry, Coulometry, Voltammetry and Amperometry.

Fundamentals of Electrochemistry: Electrical dimensions and unit, Faraday's laws of electrolysis, Theory of electrolytic dissociation, van't Hoff factor and degree of dissociation, Specific Conductance, Equivalent conductance, Equivalent conductance at infinite dilution, Variation of equivalent conductance with concentration for strong and weak electrolytes, Conductance ratio and degree of dissociation, Equivalent conductance minima, Influence of dielectric constant on conductance, Transport no., Kohlrausch's law, Application of ion conductance, Ionic mobility, Influence of temperature on ionic conductance, Ion conductance and viscosity, Drift Speed, Variation of ionic mobility with ionic size and hydrodynamic radius, factors affecting the ionic mobility for strong electrolytes, Ionic Atmosphere, relaxation effect or asymmetry effect, Electrophoretic effect, partial molar quantities (briefly), partial molar free energy and chemical potential, Electrolytes as a non ideal solution, activity coefficient, mean ionic activity, mean ionic molality, mean ionic activity coefficient, Outline of Debye Huckel theory, Debye Huckel's limiting law, variation of activity coefficient with ionic strength, Nernst equation.

Prerequisite: Chemical Principles (CHY111) and Inorganic Chemistry-I (CHY144)

❖ **CHY242: Coordination Chemistry** (4 credits: 3 Lectures + 0 Tutorial + 1 Lab) Spring

This course will focus on the basic concept of coordination chemistry and their quantification in photophysical and magnetic properties. Students will synthesize interesting transition metal based coordination complexes and perform reactions to promote the understanding of common reactions for complexation. After successful synthesis, characterisation of the synthesised materials will be performed by using analytical and spectroscopic techniques, such as thin layer chromatography (TLC), ultraviolet-visible (UV-vis), infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy. After characterization, interpretation of the results, such as extent of reaction, purity of product and photophysical property particularly colour of the coordination complexes will be learnt.

Course content

Introduction: Meaning of metal coordination and use of metal coordination in biology and materials science.

Structures of complexes: nomenclature, coordination number, bonding of organic ligands to transition metals, coordination number, linage isomerism, electronic effects, steric effects, geometry, Fluxional molecule.

Chelate and Macrocylic effect: stability, free energy, enthalpy, entropy of complexation, mimicking natural systems (chlorophyll, porphyrin, etc.) and applications.

Spectra and Bonding: Molecular orbital (MO) diagram of CO, O_2, N_2, ^{-}CN, H_2O, NH_3, BF_3, and other related ligands, Valence bond theory: Application and limitations; Crystal field theory: application and limitation; Molecular orbital theory: Application in π-bonding, electronic spectra including MLCT, LMCT, MMCT, LLCT. d-d transition, term symbol, Orgel diagram, Tanabe-Sugano diagram, and spinels chemistry.

Magnetism: Meaning of magnetism, diamagnetic, paramagnetic, ferromagnetic materials, and magnetic measurement.

Chemistry of f-block elements: Periodic trend of oxidation state, physical and chemical properties, electronic spectra, structure, and bonding.

Lab Schedule:

S. No	Experiments
1	**Expt.1-** Preparation and UV-Vis study of simple coordination complexes, such as hexaaquacobalt(II), hexaaquacopper(II), hexaaquanickel(II) ions
2	**Expt.2-** Synthesis of [Ni(disalicyaldehyde-1,2-phenylenediamine)] coordination complex
3	**Expt.3-** Characterization of [Ni(disalicyaldehyde-1,2-phenylenediamine)] coordination complex using IR, UV-Vis, NMR
4	**Expt.4-** Analysis of [Ni(disalicyaldehyde-1,2-phenylenediamine)] coordination complex
5	**Expt.5-** Synthesis of [VO(2,4-pentanedione)$_2$]
6	**Expt.6-** Characterization of [VO(2,4-pentanedione)$_2$] by using IR, UV-Vis, NMR
7	**Expt.7-** Analysis of [VO(2,4-pentanedione)$_2$]
8	**Expt.8-** Preparation and characterization of potassium trioxalatoferrate (III)
9	**Expt.9-** Synthesis of [Cr(2,4-pentanedione)$_3$]
10	**Expt.10-** Characterization of [Cr(2,4-pentanedione)$_3$] by using IR, UV-Vis, NMR
11	**Expt.11-** Analysis of [Cr(2,4-pentanedione)$_3$]
12	**Expt.12-** Synthesis of [Co(2,4-pentanedione)$_3$]
13	**Expt.13-** Characterization of [Co(2,4-pentanedione)$_3$] by using IR, UV-Vis, NMR
14	**VIVA**

Prerequisites: Chemical Principles (CHY111) and Chemical equilibrium (CHY211).

In-Depth Courses

In-depth courses provide not only advanced instruction, but also development of critical thinking and problem-solving skills and computational data analysis and modelling. Students are expected to be able to define problems clearly, develop testable hypotheses, design and execute experiments, analyse data using appropriate statistical methods, and draw appropriate conclusions, applying an understanding of all chemistry sub-disciplines. Students are also expected to be able to use the peer-reviewed scientific literature effectively and evaluate technical articles critically, learning how to retrieve specific information from the chemical literature, with the use of online, interactive database-searching tools.

❖ **CHY245: Inorganic Chemistry-II** (4 credits: 3 Lectures+ 0 Tutorial + 1 Lab) Monsoon

The course covers chemistry of p block elements.

Course content:

Chemistry of Group 13-17 Elements of the periodic table:

Group 13: Inert pair effect, relativistic effect, the reactivity of the elements, hydrides, halides, oxides and hydroxides, boron Cluster, Wade's rule.

Group 14: Occurrence and extraction, applications, physical properties reactivity of the elements, hydrides, carbides and silicides, halides, oxides and hydroxides, oxoacids and silicates, siloxanes (silicones), sulfides, nitrides, aqueous solution chemistry of group 14 elements.

Group 15: Occurrence and extraction, applications, physical properties, bonding, the reactivity of the elements, hydrides, nitrides, phosphides and arsenides, halides and oxohalides, oxides and oxoacids, phosphazenes, sulfides, and selenides.

Group 16: Occurrence and extraction, applications, physical properties, bonding, the reactivity of the elements, hydrides, metal sulfides and polysulfides, selenides and tellurides, halides, and oxohalides, oxides and oxoacids, compounds with nitrogen and aqueous solution chemistry group 16 elements.

Group 17: Occurrence and extraction, applications, physical properties, bonding, the reactivity of the elements, hydrides, oxy acids, pseudohalogens, polyhalides, interhalogen, iodine based reagent in organic transformation. Oxidation state and redox property of group elements: periodic trends in reduction potential.

Lab Schedule:

S. No	Experiments
1	**Expt.1-** Redox titration with $K_2Cr_2O_7$ a) Estimation of Fe(II) using $K_2Cr_2O_7$ solution b) Estimation of Fe(III) and Cu(II) in a mixture using $K_2Cr_2O_7$
2	**Expt.2-** Complexometric titration: Zn(II) and Cu(II) mixture
3	**Expt.3-** Gravimetry analysis a) Estimation of Ni(II) using Dimethylglyoxime (DMG) b) Estimation of Al(III) by precipitating with oxine and weighing as $Al(oxine)_3$
4	**Expt.4-** The nature of Iodine in different solvents: extend of charge transfer
5	**Expt.5-** Synthesis and characterization of *tert*-Butylamine: Borane, a Lewis acid-base adduct
6	**Expt.6-** Variable oxidation states of Tin: Preparation of Tin(IV) Iodide and preparation of Tin(II) Iodide
7	**Expt.7-** Synthesis of *hexakis*(4-nitrophenoxy)cyclotriphosphazene
8	**Expt.8-** Positive oxidation states of Iodine: Preparation of dipyridineiodine(I) nitrate
9	**Expt.9-** Friedel Craft reaction using $AlCl_3$
10	**VIVA**

Prerequisites: Chemical Principles (CHY111), Basic Organic Chemistry I (CHY122) and Inorganic Chemistry I (CHY144).

❖ **CHY311: Chemical Binding/Quantum Mechanics** (4 credits: 3 Lectures + 1 Tutorial + 0 Lab) Monsoon

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.

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_x^2 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 H_2^+, bonding and antibonding MOs, qualitative LCAO treatment of H_2 (detailed derivation not required), Basic concepts of HF and DFT.

Prerequisites: Chemical Principles (CHY111), Physics (PHY101/PHY103/PHY102/PHY104), and Mathematical methods (MAT101/ MAT103)/ Mathematics for Chemists-I (CHY103).

Co-requisite: Molecular Spectroscopy (CHY313).

❖ **CHY313: Molecular Spectroscopy** (4 credits: 3 Lectures + 1 Tutorial) Monsoon

In this course, Rotational, Vibrational, UV-Visible, Fluorescence and NMR spectroscopy methods will be taught. Chemists often adopt these techniques to identify the electronic and molecular structures of chemical and biochemical systems. Students will achieve a knowledge about the behaviour of molecular systems in presence of an external electromagnetic field in different frequency ranges. The principle along with comprehensive theories for each of the spectroscopy method will be discussed in the classes.

Course content

Introduction: Meaning of spectroscopy and use of different spectroscopic tools to understand diverse applications.

Origin of spectra: Revision of electromagnetic spectrum and Energy associated with them, Electromagnetic field, Molecular energy states and spectroscopic transitions, Factors affecting line broadening and intensity of lines, selection rules.

Rotational Spectroscopy: Rotational spectroscopy of diatomic molecules, Degeneracy of rotational levels, Effect of isotopic substitution, centrifugal distortion, Non-rigid rotator. Application of rotational spectroscopy

Vibrational spectroscopy: Infrared spectroscopy, Harmonic oscillator, Anharmonic model, vibrational-rotational spectrum, breakdown of Born-Oppenheimer Approximation, vibration of polyatomic molecules, Fourier-Transform infrared spectroscopy and its advantage, applications. Raman Spectroscopy, Classical theory of Raman scattering, Polarizability, Rule of mutual exclusion.

UV-Vis spectroscopy: Theory of UV-Vis/electronic spectroscopy: Lambert-Beer's Law, Woodward-Fieser Rules, Molecular potential energy, Molecular term symbol, Selection rules and electronic transition, Chemical analysis by electronic spectroscopy.

Fluorescence spectroscopy: Introduction to fluorescence spectroscopy: Jablonski diagram, Radiative and non-radiative rates, Frank-Condon principle, Stokes shift, solvent relaxation, solvatochromism, excimer and exciplex formation, quantum yield & life-time. Spin-orbit coupling.

Nuclear Magnetic Resonance (NMR): Theory of NMR, Spinning nucleus, effect of an external magnetic field, precessional motion and Larmor frequency, temperature effect, Boltzman distribution, origin of chemical shift and

its implication in magnetic field strength, anisotropic effect, proton NMR spectrum, carbon NMR, concept of multi-dimensional NMR, influence of restricted rotation, fluxional molecules, conformational dynamics, solvent shift, concentration and temperature effect, hydrogen bonding, theory of spin-spin splitting and coupling constants, factors influencing the coupling constant, geminal coupling, vicinal coupling, heteronuclear coupling, deuterium exchange. Rotating frame of reference, Spin-spin and spin-lattice relaxation. Pulse NMR technique.
Prerequisites: Chemical Principles (CHY111) and Physical Methods in Chemistry (CHY214).

- **CHY321: Named Organic Reactions and Mechanisms** (2 credits: 2 Lectures) Monsoon

C-C bond forming reactions and their mechanism focusing on Carbanion alkylation, Carbonyl addition and carbonyl substitution reactions, Conjugate addition reactions (1,2-addition & 1,4- addition), Reactions of alkene, alkynes and aromatics. C-N and C-O bond forming reactions and their mechanism. Glycosylation reactions. Oxidation and reduction reactions, Rearrangement reactions, Free radical reactions. Photochemical reactions and mechanism, Norrish type I and II reactions. The above reactions will be taught under some name reactions. This is an advanced level course where various name reactions are taught. This course is built on the knowledge of basic structure and bonding and various organic reactions, functional group conversions that are taught in the previous organic chemistry courses (CHY221, CHY222). This course will equip students with enough knowledge on various organic name reactions and their probable mechanisms to carry out multistep organic transformations.
Course content
C-C Bond forming reactions and Mechanism: Ring Closing Metathesis, Heck Reaction, Negishi Reaction, Suzuki Reaction, Reformatsky reaction, Ugi reaction, Morita-Baylis-Hillmann Reaction.
C-N Bond forming reactions and Mechanism: Ullmann reaction, Buchwald and Hartwig reaction, Metal free C-N bond formation reactions, Fisher Peptide synthesis, Click reaction.
C-O Bond forming reactions and Mechanism: Allan-Robinson reaction, Fisher Oxazole synthesis, Ferrier reaction, Glycosidation reaction, Sharpless asymmetric Epoxidation.
Oxidation, Reduction reactions and Mechanism: Bayer-Villeger oxidation, Dess-Martin periodinane oxidation, Swern Oxidation, Corey–Kim oxidation, Luche reduction, Birch reduction, Gribble reduction.
Rearrangement Reactions and Mechanism: Benzilbenzilic acid rearrangement, Pinacol Pinacolone rearrangement, Fries rearrangement, Amadori rearrangement, Demzanov rearrangement, Payne rearrangement, Wallach rearrangement, Ferrier rearrangement.
Conjugate addition reactions and Mechanism: Prins reaction.
Photochemical reactions and Mechanism: Norish type I reaction, Norish type II reaction.
Prerequisites: Basic Organic Chemistry-II (CHY221).

- **CHY322: Heterocyclic Chemistry** (3 credits: 3 Lectures) Spring

Heterocyclic chemistry will be discussing organic chemistry regarding the synthesis, properties, and applications of these heterocycles. These cyclic compounds with the ring containing carbon and other element, the component being oxygen, nitrogen and sulfur. Also heterocyclic compounds as natural products will be discussed and to advance the knowledge of heterocyclic structures.

Course content

Introduction: Definition of terms and classification of heterocycles, Functional group chemistry (imines, enamines, acetals, enols, and sulfur-containing groups), Synthesis of pyridines

Intermediates used for the construction of aromatic heterocycles: Synthesis of aromatic heterocycles, Examples of commonly used strategies for heterocycle synthesis, Carbon–heteroatom bond formation and choice of oxidation state

Pyridines: General properties, electronic structure, electrophilic and nucleophilic substitution of pyridines, metallation of pyridines.

Pyridine derivatives: Structure and reactivity of oxy-pyridines, alkyl pyridines, pyridinium salts, and pyridine *N*-oxides

Quinolines and isoquinolines: General properties and reactivity compared to pyridine, Electrophilic and nucleophilic substitution quinolines and isoquinolines, general methods used for the synthesis of quinolines and isoquinolines.

Five-membered aromatic heterocycles: General properties, structure and reactivity of pyrroles, furans and thiophenes, methods and strategies for the synthesis of five-membered heteroaromatics, electrophilic substitution reactions of pyrroles, furans and thiophenes, strategies for accomplishing regiocontrol during electrophilic substitution, Metallation of five-membered heteroaromatics and use the of directing groups

Indoles: Comparison of electronic structure and reactivity of indoles to that of pyrroles, Fisher and Bischler indole syntheses, reactions of indoles with electrophiles, Mannich reaction of indoles to give 3-substituted indoles (gramines), modification of Mannich products to give various 3-substituted indoles, synthetic strategies to access natural products and pharmaceutical drugs based on indoles

Azoles (1,2 and 1,3-): Structure and reactivity of 1,2- and 1,3-azoles, synthesis and reactions of imidazoles, oxazoles and thiazoles, Synthesis and reactions of pyrazoles, isoxazoles and isothiazoles.

Student presentation: Topic will be suggested by the instructor.

Prerequisites: Basic Organic Chemistry-II (CHY221) and Named Reactions and Mechanisms (CHY321).

❖ **CHY323: Organometallic Chemistry** (3 credits: 3 Lectures) Monsoon

This course includes the concept of organometallic chemistry (definition) and how organometallic chemistry is different from coordination chemistry. In first half we will cover origin of organometallic chemistry, 18 electron rules, CO, NO, PR_3, alkene, alkyne, carbene, benzene, H_2, O_2 and N_2 as ligand. In second half we will cover some example of organometallic catalyst, ferrocene chemistry, organometallic chemistry of p-block elements and reaction mechanism etc.

Course content

Introduction of organometallic chemistry: History of organometallic chemistry; Fundamentals of coordination and organometallic chemistry in terms of MO approach; 18 electron rules and its violation; M-M bonding.

Metal carbonyl chemistry: Bonding modes (IR stretching frequency); Reactions of metal carbonyls (activation, nucleophilic addition); Metal Carbonyl *vs*. metal nitrosyls *vs*. metal cyanidies; Linear nitrosyl *vs*. bent nitrosyls.

Phosphine as spectator ligands: Tolman con angle *vs*. basicity (IR stretching frequency)
Alkene and alkyne as ligand: Structure and bonding of Zesis salt, Bonding in terms of molecular orbital.
Carbene chemistry: Fisher *vs.* Schrock carbene, stability and reactivity of singlet and triplet carbene (e.g. Li_2C vs H_2C vs F_2C etc.); Synthesis and application; N-heterocyclic carbene, carbene *vs*. carbine (introductory level); Zero-electron ligand, delta bonding.
Alkyl, aryl and ligands with higher heptacity: Heptacity; MO approach; Cyclic and acyclic polyenyl pi-bonded ligands; Sandwich compounds; Chemistry of Cp*; Basic chemical reactions of ferrocene; 1,3-butadiene, cyclobutadiene, cycloheptatriene, cyclooctatetraene and benzene as ligand.
Reaction mechanism: Oxidative addition, Reductive elimination, Migration, Insertion, beta H elimination; Trans effect *vs*. Trans influence: mechanistic approach
C-H activation: Introduction, C-H functionalization *vs*. C-H activation; Importance; Classification; Organometallic C-H activation *vs*. biological C-H activation; Present research status.
Synthetic Applications of Complexes Containing Metal-Carbon Sigma-Bonds:

- Homogeneous catalysis by soluble transition metal complexes: Hydroformylation; Hydrogenation; Olefin Metathesis; Olefin polymerization, detailed kinetic and mechanistic study.
- Catalysis: Heterogeneous catalysis; Terminology in catalysis, Application of chiral phosphine ligand in catalysis.
- Organometallic chemistry of p-block elements.

Prerequisites: Coordination Chemistry (CHY242).

❖ **CHY342: Chemistry of Solids and Surfaces** (3 credits: 3 Lectures) Spring

In this course, the students will get to know the chemistry behind the formation of solids and on their surfaces, the kind of bonding involved and the available techniques to characterize them. Through this course students will also learn how to interpret various chemical structures of solids and their surfaces. Students will further understand crystallographic terminology, selected diffraction theory, nomenclature at surfaces, reconstruction and relaxations at surfaces and how to determine the surface structure. They will also realize the wide range of chemical information available from diffraction-based techniques. Further the students will learn about different surface phenomena such as adsorption, catalysis, work function, and basics of the electronic, magnetic, and optical properties, and their relevance to nanomaterials.

Course content

Introduction to Solid State Chemistry: Classification of solids based on different binding forces: molecular, ionic, covalent and metallic solids, amorphous and crystalline solids.
Crystal Chemistry: Introduction to crystal Cchemistry, unit cells and crystal systems, Bravais lattices and lattice spacing, planes, Miller indices, reciprocal lattices, crystal densities and packing efficiency, crystallographic notations, Symmetry: point group and space group.
Bonding in Solids: Overview on Bonding, Ionic, Covalent, Metallic, van der Waals and Hydrogen Bonding, Intermolecular Forces, Lattice Energy.

Crystalline Materials: Properties of X-Rays, X-Ray Diffraction Techniques, Point & Line Defects, Line, Interface & Bulk Defects

Solid State Properties: Optical properties, Electrical properties, Thermal properties.

Introduction to the Chemistry of Surfaces: Surface structure (Nomenclature, Surface unit cell, Relaxation and reconstruction at surfaces and its relevance to nanomaterials, How to characterize atomic structure at surfaces), Basics of different phenomena at surfaces (Surface energy**,** Electronic structure, 2D Brillouin zone, photoemission**,** Work function**,** Magnetic properties and relevance to nanomaterials**,** Optical properties**,** Adsorption and catalysis**,** Two dimensional structures.

Prerequisites: Chemical Principles (CHY111) and Physical Methods in Chemistry (CHY214) or Physics (PHY101/102/103/104).

❖ **CHY351: Macromolecules** (3 credits: 3 Lectures) Monsoon

The course is designed to assist a transition of the knowledge acquired by students during school level to university level. In this course we will learn about cellular macromolecules such as carbohydrates, nucleic acids, and proteins. The chemistry and biochemistry associated with these macromolecules will be discussed with examples. The goal is to learn about these important natural macro molecules, not only from a structural but from an atomic point of view as well. We will talk about the chemistry associated with these molecules including nomenclature, stereochemistry, associated chemical reactions and their importance. Classes will be through a combination of lectures, presentations and assignments.

Course content

Introduction of Macromolecules

Carbohydrates: Introduction, function and importance in chemistry and biology, class of carbohydrates monosaccharides (definitions and functions, Nomenclature, Fischer Projections and D/L notation, Open chain and cyclic structure of pentose, hexose sugars, determination of configuration/ absolute, mutarotation, ascending and descending in monosaccharides, chemical reactions of monosaccharides), Oligosaccharides (examples and functions), Polysaccharides (Homo and hetero polysaccharides, examples and their functions (Starch, Glycogen, Dextran, Cellulose, Chitin, Agar Galactosan, Hyaluronic acid)).

Glycoconjugates: Proteoglycans, Glycoproteins, Structural and Functions of glycoproteins

Nucleic Acids (DNA and RNA): Introduction of nucleic acids, classes of nucleic acids, building-blocks Purine and Pyrimidine bases, sugars and phosphates, structures, examples and functions of nucleosides & nucleotides, structures of polynucleotides, forces for stabilities of base-pairing, discovery of DNA and structure of DNA, Watson and Crick's Model, minor and major grooves in DNA, types (A, B and Z-DNA and their biological relevance).

Amino acids, peptide and proteins: Amino Acids (name, structures, three letter code, one letter code), Common features of amino acids (AA), Number of carbons in amino acids, classification (D, L) and configurations of amino acids, classification of AA side chains by chemical properties (Polar, non-polar, ionic amino acids), acid base properties of amino acids (pKa calculations),Ionization of AAs (Zwitter ion, isoelectric point and electrophoresis), Peptide, oligopeptides structures and proteins, reaction of amino acids N terminus and C terminus Ester of carboxylic group, acetylation of amino group, Complexation with Cu^{2+} ions, Ninhydrin test, Post translational modifications (phosphorylation, glycosylation etc.), preparation of amino acids, Strecker synthesis, Gabriel phthalimide synthesis.

Protein Structure and quick overview of primary, secondary, tertiary, and quaternary structure, structure determination of peptides. Synthesis of simple dipeptides by N-protection (t-butoxycarbonyl and phthaloyl), C-activating group and Merrifield solid phase synthesis.

Prerequisites: Basic Organic Chemistry-II (CHY221).

Electives

- **CHY326: Stereoelectronic Effects in Organic Chemistry** (3 credits: 2 Lectures + 1 Tutorial) Spring

To design new organic materials, it is absolutely essential to have detailed understanding of the structure, energies and reactivities of the newly design molecules and stereoelectronic effects play crucial role to determine these factors. A comprehensive overview of classical as well as modern stereochemical models and their application will be presented during this course. A multidimensional approach will be discussed for deeper understanding of this effect. Primary aim of this course is to answer how stereoelectronic effect is applicable to organic chemistry for broader and deeper understanding of inherent reactivities and properties of organic molecules. Major attention will be paid to make a bridge between the classical and modern stereoelectronic models to explain the stereochemical outcome of organic reactions.

Course content

Introduction: Historical perspectives and recent application stereoelectronic effect.

Role of orbital interaction on reactivity: bond formation without bond breaking and bond formation with bond breaking.

Factors controlling effective orbital overlap: hybridization, orbital size, distortions, steric effects, directionality, ionic character and charge distribution, electronic counts, isovalent vs sacrificial conjugation and hyperconjugation.

Stereoelectronics of supramolecular interactions: FMO interactions in the intramolecular complex and H-bonding in enzymes and supramolecular interactions with π systems.

Combined computational and experimental approach to study stereoelectronic effect:

General trends of donors and acceptors: antiperiplanarity & polarization, hybridization & orbital energy effect.

From orbital interaction to conformational analysis: alkanes, carbonyls & ester and related carbonyls, amides, vinyl ether and enamines,

Remote stereoelectronic effect: homoconjugation, homoanomeric effect, cross hyperconjugation, through space interaction, symmetry and co-operative effect.

Application of stereoelectronic effects in reaction design: application of static and dynamic stereoelectronic effects, catalyst design, in enzyme catalyzed reaction in bioorganic chemistry.

Probing stereoelectronic effects with spectroscopic methods: Bohlmann effect, intramolecular vesion of Bohlmann effect, diamagnetic effect, anomeric effect, paramagnetic effect, Perlin effects, reverse Perlin effects, through-space interactions, and umpolung effect-NMR consequences of positive hyperconjugation.

Prerequisites: Basic Organic Chemistry-II (CHY221) and Chemistry of Carbonyl Compounds Chemistry (CHY222).

❖ **CHY332: Informatics & Machine Learning** (3 credits: 2 Lectures + 3 h computer lab) Spring

This course and the associated computer lab deal with Molecular Modelling and Cheminformatics, applied to the search for new drugs or materials with specific properties or specific physiological effects (*in silico* Drug Discovery). Students will learn the general principles of structure-activity relationship modelling, docking & scoring, homology modelling, statistical learning methods and advanced data analysis. They will gain familiarity with software for structure-based and ligand-based drug discovery. Some coding and scripting will be required.

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.

Representation of Chemical Structure and Similarity: Sequence Descriptors, Text mining, Representations of 2D Molecular Structures: SMILES, Chemical File Formats, 3D Structure, Descriptors and Molecular Fingerprints, Graph Theory and Topological Indices, Progressive incorporation of chemically relevant information into molecular graphs, Substructural Descriptors, Physicochemical Descriptors, Descriptors from Biological Assays, Representation and characterization of 3D Molecular Structures, Pharmacophores, Molecular Interaction Field Based Models, Local Molecular Surface Property Descriptors, Quantum Chemical Descriptors, Shape Descriptors, Protein Shape Comparisons, Motif Models, Molecular Similarity Measures, Chemical Space and Network graphs, Semantic technologies and Linked Data.

Mapping Structure to Response: Predictive Modeling which includes Linear Free Energy Relationships, Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) 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, Model Domain of Applicability.

Data Mining and Statistical Methods which includes Linear and Non-Linear Models, Data preprocessing and performance measures in Classification & Regression, Feature selection, Principal Component analysis, Partial Least-Squares Regression, kNN, Classification trees and Random forests, Cluster and Diversity analysis, Introduction to kernel methods, Support vector machines classification and regression, Introduction to Neural Nets, Self-Organized Maps, Deep Neural Networks, Introduction to evolutionary computing, Deep Learning and Convolutional Neural Nets, Genetic Algorithms, Data Fusion, Model Validation, Best Practices in Predictive Cheminformatics.

Prerequisites: Basic Organic Chemistry-I (CHY122), Basic Statistics (MAT284/MAT084), Programming (CHY114/ BIO101/MAT110/PHY105/CSD101)

❖ **CHY 348: Bio-inorganic Chemistry** (3 credits: 3 Lectures) Spring

This course includes origin of bioinorganic chemistry, uses of metal ions in life, analytical techniques involved to determine reactive intermediates and to predict mode of action, reaction mechanism and bio-mimetic catalyst designing.

Course content:

1. General discussion about bioinorganic chemistry.
2. Biological important elements, Biological ligands.
3. Alkali and alkaline earth metal in biology: Role of Na, K (Na-K pump, chelate chemistry, SHAB theory); Mg (ATP hydrolysis and chlorophyll) and Ca.
4. Zn(II) as nature's lewis acid: Hydrolase enzyme, Zn containing hydrolase enzyme e.g. Carbonic anhydrases (CA), therapeutic application of CA inhibitors; carboxypeptidase and its classification.
5. Importance of Oxygen, Great oxygenation event.
6. Iron based chemistry in nature; Iron metabolism: Iron transport, Iron storage; Iron cycle.
7. Oxygen utilization: (i) Oxygen transport and storage (Hemoglobin *vs*. Myoglobin) (ii) Oxidases enzyme: Cytochrome c oxidase, Electron transport chain, Cytochrome c oxidase vs. Cytochrome in respiratory cycle; electron transfer reaction in biology; (iii) Oxygenase: Cyt P450: Reaction mechanism; (iv) Peroxidase: HRP; (v) Importance of metal-oxo species, role of axial ligand for stabilizing metal-oxo species and controlling the reactivity, effect of electronics on the reactivity of oxo intermediate, oxo wall theory; (vi) Bio-mimetic catalyst designing.
8. Organophosphate compounds, Nerve reagent, role of Zinc in phosphate hydrolysis, alkaline phosphatase and acid phosphatase enzyme, model compound for nerve reagents destruction.
9. Fe-S protein and its role, Hydrogenase enzyme, role of π-acid ligand.
10. Cu containing protein and enzyme: Hemocyanin (spectroscopic characterization of oxygenated hemocyanin), Blue Cu protein, Superoxide dismutase (role of Cu and Zn in SOD).
11. Importance of Mn in nature: Why nature use manganese in photosynthesis? Importance of water oxidation in photosynthesis, O-H bond activation, solar energy conversion; Mn containing SOD.
12. Mo-containing enzyme: Nitrogenase, nitrogen cycle.
13. V (e.g. Haloperoxidase), Co (e.g. Vitamin B12), Ni (e.g. Urease, Ni containing SOD) containing enzymes/ bio-molecules.
14. Se containing enzyme (e.g. Glutathione peroxidase).

Prerequisites: Coordination Chemistry (CHY242), Organometallic and Bio-inorganic Chemistry (323)

❖ **CHY352: Advanced Biochemistry** (3 credits: 3 Lectures) Spring

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

Course content

General Introduction on Biomolecules: Carbohydrates, Proteins, Nucleic Acids, Lipids, Enzymes and Vitamins (in brief)

Carbohydrates: Structure and Functions, metabolism, Kreb's Cycle and Glycolysis.

Proteins: Properties, Structure and Functions, Protein Sequencing, why does sequence matter? Protein sequencing from scratch, End group analysis, Cyanogen bromide method, Sanger's method, and Dansyl chloride method, Edman degradation , De novo peptide sequencing, Sequence by Mass Spectrometry (MALDI, ESI-MS, Tandem MS).

Nucleic Acids: Introduction of Nucleic acids, Gene expression, Genetic Code, Translation (DNA-Protein), How peptides are synthesized? Chemical reactions involved in peptide synthesis, DNA Sequencing, Sanger dideoxy method for sequencing, Maxam Gilbert method, DNA chemistry, DNA damage, Methylation and demethylation, Oxidative DNA damage, DNA-DNA crosslinks, DNA-Protein crosslinks, Mutagenesis, Diseases and carcinogenesis, PCR, RT-PCR techniques, DNA Finger printing (Agarose gel electrophoresis), Application of PCR such as Forensics, Relationships, Medical Diagnostics

Lipids: Fats (properties and functions), Fatty Acids, Classes of Lipids, Nomenclature of fatty acids Examples of diff. Lipids, Phospholipids, Steroids, Beta Oxidation mechanism

Enzymes: Co-factors, Co-enzymes, Apo-enzyme, Halo enzymes, Factors effecting Enzymes (Con., pH, T), Nomenclature, Mechanism of Enzymes, Biosynthesis of cofactors, NAD+-NADPH, Biosynthesis of Niacin (Vitamin B3), FAD-FADH-FADH2, Thiamine pyrophosphate TPP, Enzyme assay in Diagnostic Medicine

Hormones and Vitamins: Classifications, Examples and Functions

Prerequisites: Macromolecules (CHY351) or Biochemistry (BIO204) or Cell Biology and Genetics (BIO201)

❖ **CHY 356: Polymers** (3 credits: 3 Lectures) Monsoon

The chemistry of polymers, their synthesis and characterization will form the subject matter of this advanced course, which will follow a case-study approach. Students will be expected to apply their knowledge to a real-world problem of their choice. How do changing demands in society lead to polymer invention? How are monomers bonded in nature to form our body's building blocks? How do scientists mimic nature in labs? How does the several-fold change in molecular weight from monomer to polymer result in different sets of properties? Most of the polymeric materials around us are synthesized in different ways, depending upon end usage. This course will help to understand the need and importance of polymers in today's world. Interesting chemical aspects of synthesis of polymeric architectures from small molecules will be explored.

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)

Prerequisites: Basic Organic Chemistry-II (CHY221).

❖ **CHY413: Applications of Analytical Techniques** (3 credits: 3 Lectures) Monsoon

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

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: Basis 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.

Mass spectroscopy technique: Principle and applications, different mass spectroscopy methods (ESI, MALDI, LCMS, GCMS), isotopic distribution.

Problem solving: Solving unknown structures using above spectroscopic techniques.

Pre-requisites: Basic Organic Chemistry-II (CHY221), Chemistry of Carbonyl Compounds (CHY222).

❖ **CHY424: Medicinal Chemistry** (3 credits: 3 Lectures) Spring

In this course we will address various issues regarding drugs and its role inside a cell. We will learn what are drugs and their different types? How do drugs work? What causes side effects? How do drugs become resistance? These and other questions will be considered in this course. We will learn the chemistry and biochemistry necessary to understand the mechanism of drug action and the process of drug discovery and development. Students will investigate what is known about active ingredients in natural remedies. Social, ethical and economic issues related to drugs will be addressed. Instruction will be through a combination of group discussions, reading assignments, projects, video presentations and lectures. Students are expected to do library research, read papers, and present discussion in class.

Course content

Drugs and the body: What are drugs? What are the common drug targets? Why do they work? How are drugs transported?

- Types of Drugs and Drug Targets: DNA Damaging agents, Enzymes, mechanism based inhibitors, covalent inhibitors, Receptors
- Drug Discovery and optimization: Generation of lead compounds, Lead Optimization, Preclinical studies Clinical trials

Drug Metabolism: Phase I, Cytochrome P450, Aldehyde dehydrogenase, Monoamine oxidase

Phase II (GST, UGT)

- Transporters Drug toxicity: Reactive intermediate, Adverse effects, Drug-drug interaction, Polymorphism and its effect on drug action/toxicity: Structure-activity relationships
- Mechanism of action: Painkillers and opioids (e.g. morphine), Antidiabetic, Antibiotics, Anticancer, NSAIDS, Statins, Blood Thinners, Antacids/Proton pump inhibitors, Antivirals, Antidepressant/antipsychotic
- Synthesis and biosynthesis of drugs, Combinatorial chemistry

Prerequisites: Macromolecules (CHY351) or Biochemistry (BIO204) or Cell Biology and Genetics (BIO201) or Advanced Biochemistry (CHY352).

❖ **CHY409: Strategies for problem solving** (3 credits: 3 Lectures + 0 Tutorial + 0 Lab) Monsoon

The course focuses on the problem-solving strategies for inorganic, organic and physical chemistry taught in the undergraduate as well as postgraduate level. In this course, strategies for solving chemical problems will be taught through lecture, tutorial and home assignments. The courses will provide a journey of various aspects of chemistry and utilize them on how to approach and answer several problems on organic, inorganic and physical chemistry syllabuses. This course will also cover problem solving strategy in nanoscience and technology, bioorganic chemistry including carbohydrates, proteins, nucleic acids, catalysis and supramolecular chemistry. This course will offer students techniques to solve problems related to organic, inorganic and physical chemistry for the competitive examinations at the masters and PhD entrance examinations, nationwide. It will help students to get motivated in national exam and develop skills in academia. Furthermore, this course will be an excellent steppingstone into their higher education.

Course Content

Organic Chemistry: 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.

Inorganic Chemistry: 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.

Physical Chemistry: 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.

Prerequisites: Inorganic courses: CHY241, CHY323, CHY242, CHY245, CHY553; Organic Course: CHY321 and CHY322; Physical course: CHY211, CHY212, CHY214, CHY241, CHY311.

❖ **CHY444: Nanotechnology and Nanomaterials** (3 credits: 3 Lectures) Spring

The next few years will see dramatic advances in atomic-scale technology. Molecular machines, nanocircuits, and the like will transform all aspects of modern life - medicine, energy, computing, electronics and defense are all areas that will be radically reshaped by nanotechnology. These technologies all involve the manipulation of structures at the atomic level - what used to be the stuff of fantasy is now reality. The economic impact of these developments has been estimated to be in the trillions of dollars. But, as with all new technologies, ethical and legal challenges will arise in their implementation and further development. This course will examine the science of nanotechnology and place it in the larger social context of how this technology may be, and already is, applied. Underlying physical science principles will be covered in lecture sessions and students will read articles from current news sources and the scientific literature. There will be presentations on scientific literature on topics of student interests, to examine the science and applications of a well-defined aspect of nanotechnology of their choosing. Lecture material will focus on the principles behind utility of designed nanostructures for many applications.

Course content

Introduction: Fundamental study of materials in nanosize domain, history of nanomaterials

Bulk *vs*. Nano: Nanosized metals and alloys, semiconductors, a comparison with respective bulk materials.

Methods of preparation of nanomaterials: Chemical *vs*. physical methods (Ball Mixing, Melt mixing, sputtering, Laser ablation, electron evaporation, Thermal evaporation).

Chemical methods: Top down and Bottom-up approaches, Physical and chemical methods, Nucleation and growth of nano systems; self-assembly, Chemical vapor deposition; sol-gel method, colloidal method, Spray pyrolysis; Annealing, Calcination; Synthesis of metal nanoparticles by colloidal route; Synthesis of Semiconductor Nanoparticles: Quantum Dots; Synthesis of semiconductor ZnS; Synthesis of Quantum Dots; Biological methods (Green synthesis Using microbes and plants).

Different types of nanomaterials: Zero dimension (0D), one dimension (1D), and two dimensional nanostructures (2D). Carbon nano-architectures: Fullerene, SWNT, MWNT, Graphene, nanodiamonds, etc.

Properties: Quantum confinement effect, Surface area to volume ratio, surface energy, mechanical, thermal, optical, magnetic, electrical and electronic properties.

Characterization of nanomaterials: Characterization Techniques: Spectroscopic/Optical methods; UV-VIS, Dynamic Light Scattering; (DLS), Raman, IR, XRD, Particle; tracking, Laser Diffraction; Microscopic characterization: SEM, TEM, AFM.

Applications: Nano-machines, solar cells, coatings, MEMS, nano-medicine, sensors, magnetic storage devices, miscellaneous, drug delivery and diagnostics.

Prerequisites: Chemical Principles (CHY111) and Chemistry of Solids and Surfaces (CHY342).

❖ **CHY471: Materials for Energy** (3 credits: 3 Lectures) Monsoon

Fundamental understanding of the structure-composition-performance relationships of energy materials. Fabrication and evaluation of prototype clean energy conversion & storage devices (lithium batteries, Perovskite based solar cells, supercapacitors, and fuel cells).

Course content

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.

Prerequisites: Electrochemistry (CHY241).

❖ **CHY456: Food Chemistry** (3 credits: 3 Lectures) Spring

Food chemistry is the study of chemical processes and interactions of all biological and non-biological components of foods. The biological substances include meat, poultry, lettuce, beer, and milk as examples. It is similar to biochemistry in its main components such as carbohydrates, lipids, and protein, but it also includes areas such as water, vitamins, minerals, enzymes, food additives, flavours, and colours.

Course Content

Introduction: Introduction to food, the evolution of food, function of foods, balanced diet, cooking methods.

Water: Definition of water in food, the structure of water and ice, types of water, sorption phenomenon, water activity and packaging, water activity and shelf-life.

Food lipds: Edible fats and oils - classification and chemical composition, reactions involved during deep frying of food.

Food proteins: Nature of food proteins (plant and animal proteins), reactions involved in processing and reactions with alkali, enzyme catalyzed reactions involving hydrolysis and proteolysis, process of texturization of proteins.

Food enzymes: Hydrolases, lipases and other important enzymes in food, enzymes in food processing, industrial uses of enzymes

Browning reactions in food: Enzymatic browning, non – enzymatic browning: maillard reaction, caramelization reaction, ascorbic acid oxidation

Food carbohydrates: Important polysaccharides (starch, glycogen, cellulose, pectin, hemicellulose, gums), chemical reactions of carbohydrates –oxidation, reduction, with acid &alkali, modified celluloses and starches and enzymatic degradation of polysaccharides

Minerals in foods: Major and minor minerals, trace elements in eggs, cereals & cereal products, vegetables and fruits, metal uptake in canned foods, toxic metals

Natural food pigments: Introduction and classification, food pigments (chlorophyll, carotenoids, anthocyanins and flavonoids, beet pigments, caramel)

Food additives: Vitamins, amino acids, minerals, aroma compounds in food, flavor enhancers: monosodium glutamate, nucleotides, sugar substitutes (sorbitol, saccharin, cyclamate) and food colours.

Cereals and cereals products: Individual constituents – proteins, lipids, carbohydrates and vitamins in cereals flour and their relationship in dough making, type of flours for bread making and confectioneries and influence of additives, physical, chemical changes during baking and determination of gluten and starch content in flour

Legumes: Classification, composition and physicochemical properties.

Vegetables and fruits: Classification, general composition, chemical changes during ripening and storage

Jams, Jellies and Pickles: Classification, composition and preservation.

Prerequisites: Basic Organic Chemistry-I (CHY122) and Macromolecules (CHY351) or Advanced Biochemistry (CHY352) or Biochemistry (BIO204).

❖ **CHY 522: Informatics and Drug Discovery** (3 credits: 2 Lectures + 0 Tutorial + 1 Lab (2 hour)) Spring

This course will introduce he fundamental interactions in protein-drug binding to the students and will cover the computational and bioinformatics tools to identify such interactions. Course will also provide hands-on applications to identify such interaction during via lab and practical classes.

Course Content

Introduction: Drug Discovery in the Information-rich age, Applications potential of Bioinformatics and Cheminformatics.

Representation of Chemical Structure and Similarity: Sequence Descriptors, Representations of 2D Molecular Structures: SMILES, Chemical File Formats, 3D Structure, Descriptors and Molecular Fingerprints, Substructural Descriptors, Physicochemical Descriptors, Descriptors from Biological Assays, Representation and characterization of 3D Molecular Structures, Pharmacophores, Molecular Interaction Field Based Models, Local Molecular Surface Property Descriptors, Quantum Chemical Descriptors, Shape Descriptors, Protein Shape Comparisons, Motif Models.

Mapping Structure to Response and Predictive Modeling: Linear Free Energy Relationships, Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) Modeling, Ligand-Based and Structure-Based Virtual High Throughput Screening, 3D Methods - Pharmacophore Modeling and alignment, ADMET Models, Activity Cliffs, Model Domain of Applicability.

Structure Based Computer Aided-Drug Design: Preparation of Target Structure, Comparative modelling, Model Refinement and evaluation, Binding Site Detection and Characterization, Geometric Method for the Binding site detection, Energy based approached for the binding site detection, Binding pocket matching.

Application of Bioinformatics and Cheminformatics for Drug Designing: Molecular Docking, Scoring Functions for Evaluation of Protein-ligand Complexes, End point and Alchemical Method of Binding free energy, Predicting protein structure using Comparative Modelling, Ensemble Based Approach to Map Druggable site, Evolutionary trace for prediction and Redesign of Protein Sites.

Prerequisites: Basic Organic Chemistry-I (CHY122), Basic Organic Chemistry-II (CHY221), Mathematics for Chemists-I (CHY103), Mathematics for Chemists-II (CHY104).

❖ **CHY 542: Supramolecular Chemistry** (3 credits: 3 Lectures) Spring

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.

Course Content

Non-covalent 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, π•••π interactions, Hydrophobic effect.

Aromatic-Aromatic interactions: Benzene crystals, edge-to-face vs. π•••π stacking interactions, N-H•••π interactions, sulfur-aromatic interactions, Benzene-hexafluoro-benzene π-stacking.

Supramolecular Host-guest chemistry: Receptors, Lock and Key analogy, Binding constant analysis

Supramolecular Artificial Receptors: (a) Cation Binding Hosts -Podand, Crown Ether, Cryptand, Nomenclature, Selectivity, Calixarenes. (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.

Solid-State Chemistry: Metal Organic Frameworks (MOFs), Covalent Organic Frameworks

Supramolecular catalysis and reaction in confined environment: Definition, H-bonded cages for catalysis, Self-assembling coordination cages and their uses in encapsulations and catalysis

Transport processes: Dynamic Combinatorial chemistry

Stimuli responsive solids: Topochemical [2+2] cycloadditions in cinnamic acids under light, Topochemical photopolymerization in crystals

Biological supramolecular systems: Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly.

Supramolecular Chemistry in Biology: Membranes, Macrocyclic systems, Photosynthesis, Oxygen transport, Enzymes, Heme analogues.

Prerequisites: Coordination Chemistry (CHY242), Macromolecules (CHY351)

- **CHY 548: Frontiers in Inorganic Chemistry** (4 credits: 3 Lectures + 0 Tutorial + 1 Lab) Spring

The course focuses on the fundamental and advanced topics of inorganic chemistry. This course is also complemented with futuristic laboratory experiments which will help students to learn advanced laboratory techniques, therefore, it would help for 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 d^n ions, splitting of d^n 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, $d^* \leftarrow d$ transition

Magnetochemistry: 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.

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 hetero-polyoxometalates with respect of V, Mo and W: Syntheses, reactions, structures, uses. 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.

Lab Schedule:

S. No.	Experiments
1	**Expt.1-** Rhodium Rainbow: ligand field effects of dirhodium tetraacetate.
2	**Expt.2-** Determination of Δ_0 in Cr(III) complexes and spectrochemical series.
3	**Expt.3-** The synthesis and characterization of Ferrocene and its derivatives.
4	**Expt.4-** Synthesis of compound containing Metal-Metal Quadrupole Bonds and assignment of d* ← d transition.
5	**Expt.5-** Synthesis of a selected Metal-organic Framework (MOF) and characterization.
6	**Expt.6-** Preparation of trans-dichloro-bis(ethylenediamine)cobalt(III) chloride and cis-trans interconversion.
7	**Expt.7-** Synthesis, Optical Resolution of $Co(en)_3^{3+}$.
8	**Expt.8-** The Preparation of tetraphenylporphyrin and its Metal Complex, comparison of molar extinction coefficient.
9	**Expt.9-** Preparation and Analysis of Potassium Trisoxalatoferrate(III) Trihydrate and photochemistry.
10	**Expt.10-** NMR Investigation of Molecular Fluxionality: Synthesis of Allylpalladium Complexes.

Prerequisites: Inorganic Chemistry-II (CHY245) and Coordination Chemistry (CHY242).

Co-requisites: Organometallic (CHY323).

B.Sc. (Research) Chemistry & Minor in Chemistry

Recommended Semester-wise Plan

Font: Black (all), Blue (PCBM/PCM), Brown (PCB)

Semester	Course	Course Title	L:T:P	Prerequisites	Credits Major
1 (MSN)	CHY103	Mathematics for Chemists-I	3:1:0	None	9+5=14 9+6 = 15
	CHY111	Chemical Principles	3:1:1	None	
	PHY101/ PHY103/ PHY255	Introductions to Physics-I/Fundamentals of Physics-I/ Introduction to Biophysics	3:1:1 3:0:0	None	
	BIO201*	Cell biology and Genetics*	2:0:1	PCB at 10+2	
2 (SPR)	CHY104	Mathematics for Chemists-II	2:2:0	None	14+8= 22 14+4= 18
	CHY114	Molecular modelling#	1:0:1	None	
	CHY122	Basic Organic Chemistry-I	2:1:1	CHY111	
	CHY144	Inorganic Chemistry-I	2:1:1	CHY111	
	PHY102/ PHY104/ PHY108	Introductions to Physics-II/Fundamentals of Physics-II/ Physics for Life	3:1:1 3:1:0	None	
	BIO113*	Essentials of Biology*	2:0:1	non-PCB at 10+2	
3 (MSN)	CHY211	Chemical Equilibrium	3:0:1	CHY111	17
	CHY214	Physical Methods in Chemistry#	2:0:1	CHY111	
	CHY221	Basic Organic Chemistry-II	2:1:1	CHY122	
	CHY241	Electrochemistry	2:0:0	CHY111, CHY144	
	CHY245	Inorganic Chemistry-II	3:0:1	CHY111, CHY144	
4 (SPR)	CHY212	Chemical Applications of Group Theory	3:0:0	CHY111, MAT103/CHY103	11
	CHY222	Chemistry of Carbonyl Compounds	2:1:1	CHY122, CHY221	
	CHY242	Coordination Chemistry	3:0:1	CHY111, CHY122, CHY144	
5 (MSN)	CHY311	Chemical Binding	3:0:1	CHY111, PHY101/103/102/104, MAT101/103/CHY103; CHY313	16
	CHY313	Molecular Spectroscopy	3:1:0	CHY111, CHY214	
	CHY 321	Named Organic Reactions and Mechanism	2:0:0	CHY221	
	CHY323	Organometallic Chemistry	3:0:0	CHY242	
	CHY351	Macromolecules	3:0:0	CHY221	
6 (SPR)	CHY322	Heterocyclic Chemistry	3:0:0	CHY221, CHY321	6+6 = 12 6+6+3 = 15
	CHY342	Chemistry of Solids and Surfaces	3:0:0	CHY111, CHY214 or PHY101/102/103/104	
	CHYXYZ	Electives	3:0:0	†	
	CHYXYZ	Electives	3:0:0	†	
	CHYXYZ	Electives	3:0:0	†	
7** (MSN)	CHY498	Senior Project	0:0:6	None	6+3 = 9
	CHYXYZ	Electives	3:0:0	†	
8 (SPR)	CHY499	Senior Project	0:0:6	None	6+3 = 9
	CHYXYZ	Electives	3:0:0	†	
Graduation		**Total Credits**			**110**

*BIO113/BIO201: any one course

2h lab

† specific to course

**CHY400 Colloquium (1 credit needs to be taken)

Future courses

❖ **CHY 354: Biochemical Toxicology** (3 credits: 3 Lectures)

Course content

- General Principals of toxicology
- Classes of toxicants
- Metabolism
- P450 and P450 catalyzed reactions
- Other phase 1 reactions
- Phase II/Conjugation reactions
- Bioactivation and Reactive intermediates
- Reaction of Chemicals with DNA
- DNA adducts and its consequences (Mutagenesis, DNA repair and Translesion DNA synthesis)
- Protein adducts
- Genetic toxicology (polymorphism)
- Molecular basis of toxicology
- Biomarkers
- Natural Products
- Cellular Oncogenesis
- Metals
- Drug induced liver damage
- Mass spectrometry and other analytical methods

Prerequisites: Macromolecules (CHY351) or Biochemistry (BIO204) or Cell Biology and Genetics (BIO201) CHY111 or Advanced Biochemistry (CHY352).

❖ **CHY412: Dynamics of Chemical Reactions** (3 credits: 3 Lectures)

The principles of chemical kinetics, as well as equilibrium and non-equilibrium statistical mechanics will be covered in this advanced course. The associated computer lab will introduce the student to classical and *ab initio* quantum molecular dynamics and Monte Carlo simulations of liquids and proteins. The techniques learned in this course will applied to substantive research projects that the students will design, execute, and present. Students will be encouraged to seek avenues for publication of their most significant results

Prerequisites: Chemical Equilibrium (CHY211), Chemical Binding (CHY311) and Macromolecules (CHY351).

❖ **CHY421: Organic Synthesis** (3 credits)

Students will gain expertise in the techniques of organic synthesis. A major project will be the development of a research proposal based on the student's own question. Background from the literature will motivate the proposal and initial experiments will be proposed.

Prerequisites: Named Organic Reactions and Mechanisms (CHY321) or Heterocyclic Chemistry (CHY322).

❖ **CHY452: Introduction to Bio-organic Chemistry** (3 credits)

Basic structure of nucleic acids, proteins, lipids and carbohydrates; biological functions and biosynthesis of precursors.

❖ **CHY453: Forensic Chemistry** (3 credits)

Chemistry for Forensic Scientists, Skills for Forensic Scientists Crime Scene Science, Aspects of Forensic Science, Application of Forensic Science Forensic Science Dissertation, Advances in Forensic Chemistry, Forensic Toxicology.

Prerequisites: Basic Organic Chemistry-II (CHY221) or Macromolecules (CHY351) or Advanced Biochemistry (CHY351) or Biochemistry (BIO204) or Cell Biology and Genetics (BIO201).