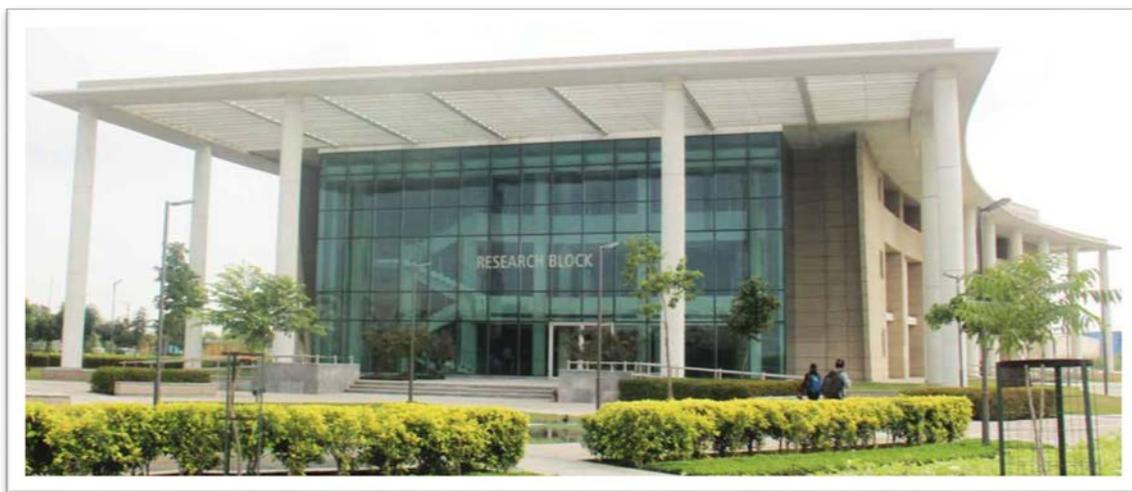


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SHIV NADAR UNIVERSITY

# DEPARTMENT OF CHEMISTRY

School of Natural Sciences



## **About the Department:**

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

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

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

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

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.

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 = 68 credits in Core Chemistry Courses (Introductory + Foundation + In-Depth) + 21 credits (Physics/Maths/Life Sciences) + 9 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 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:**

**24 credits** = 21 credits in compulsory courses (10 Introductory + 11 Foundation) + 3 credits of Chemistry In-Depth/Elective courses.

### Chemistry Course Catalogue:

The chemistry program at SNU 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.

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

### Course Summary

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 Aims

- To refresh students' basic knowledge in chemistry and advance their understanding toward the fundamentals and applied chemistry.
- To develop students' experimental skills, especially their ability to perform meaningful experiments, analyse data, and interpret observations.

### Learning Outcomes

On successful completion of the course, students will be able to refresh their knowledge on chemical principles and (i) understand the fundamentals behind the formation of atomic and molecular structures, the equilibrium and thermodynamics involved in a chemical system, various organic reactions and the basic analytical techniques to characterize chemical compounds and (ii) diagnose which mathematical elements can be used for particular analysis of data, perform experiments of the type required initially in research, use spectroscopic methods to ascertain whether the experiment was successful, read a paper and transfer that information to an experimental setup.

### Curriculum Content

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

- 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.
- Concept of Atomic Orbitals, representation of electrons move in three-dimensional space, wave function ( $\Psi$ ), 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.
- Orbital Angular Momentum ( $l$ ), Spin Angular Momentum ( $s$ ), HUND's Rule, The *aufbau* principle.
- Shielding Effect, Effective Nuclear Charge, Slater's rule
- Periodic properties elements
- 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<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, HCl, CO, NO, and CO<sub>2</sub>, degree of freedom, stretching and bending.
- l) IR spectra of different functional groups such as -OH, -NH<sub>2</sub>, -CO<sub>2</sub>H etc.
- m) UV-Vis Spectroscopy of organic molecules, Electronic Transitions, Beer-Lambert Law, Chromophores.

## **Unit-2: The Principles of Chemical Equilibrium, Kinetics and Electrochemistry:**

- Thermodynamic System & Surroundings
- 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
- Laws of Thermodynamics
  - 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
- Phase Equilibrium: Phase Diagram; Gibbs Phase Rule; Degrees of Freedom; Phases
- Chemical Equilibrium: Equilibrium Law
- 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.
- Catalysis: Homogeneous and Heterogeneous - Basics, Characteristics and Features
- Electrochemistry: Redox Reactions, Electrochemical Cells, Cell Notation, Cell Potential, Standard Reduction Potential; Nernst Equation

## **Unit-3: Organic Chemistry:**

- Introduction to organic chemistry: Examples of various organic chemicals of natural and industrial importance, Bulk vs fine chemicals
- Functional group: Types and nature
- 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)

- Substitution reactions:  $S_N1$  and  $S_N2$
- Elimination reactions: Hoffmann and Saytzeff elimination
- Name reactions: Markownikoff and Anti-Markownikoff reaction (ionic vs. free radical addition)
- Stereochemistry: definition, classification in isomerism
- Compounds containing single bonds: conformational and configurational isomerism. Isomerism in (ethane, butane and cyclohexane for mono and disubstituted)
- 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
- 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	Sugar Content of Common Drinks
4	Stoichiometry of $H_2O_2$ decomposition
	Make-up-week
5	Determination of Conc. of an Unknown coloured soln.
6	Total Hardness of Water
7	Synthesis of Nylon
	Make-up-week
8	Recycling Aluminium foil / Technique Grade
9	Analysis of Common Functional Groups
	Make-up-week
10	Synthesis of aspirin / Technique Grade
11	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	<b>Expt.1-</b> Intermolecular forces
3	<b>Expt.2-</b> Calibration of a thermometer & - Melting point and boiling point determination of unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
4	<b>Expt.3-</b> Acidity and basicity: pHmetry using a Vernier probe vs volumetric titration
5	<b>Expt.4-</b> Separation of an acidic and a neutral substance by extraction in microscale
6	<b>Expt.5 -</b> Separation of an acidic, a basic and a neutral substance by extraction in macroscale
7	<b>Expt.6 -</b> Paper chromatography for separation of amino acids
8	<b>Make-up-week</b>
10	<b>Expt.7 -</b> Thin layer and column chromatography.
12	<b>Expt.8 -</b> Synthesis and characterization: recrystallization (Schotten Baumann reaction)
13	<b>Expt.9 -</b> To find the optical rotation of a chiral molecules
14	<b>Expt.10A -</b> DSC, Rotary evaporator, Kugelrohr
15	<b>Make-up-week</b>
16	<b>Expt.10B -</b> NMR experiment

*Prerequisite:* Chemical Principles (CHY111).

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

**Course Content**

Acid-Base: Introduction, The Arrhenius theory, The Protonic theory, Theories of acids – bases : Bronsted – Lowry theory, Conjugate Acid – Base pairs, Solvent system definition, The Lux concept; Lewis theory of Acids – Bases, 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); Thermodynamic acidic parameters, Proton Sponge, Hydride Sponge, Super Acids-Hammett Acidity Function, Magic Acids/Superacids: preparation of carbocations in superacids, methane oligocondensation reaction, ethylene-methane alkylation, ethylene-ethane alkylation, conversion of isobutene into acetone and methyl alcohol; Super Base.

Ionic equilibrium

- A. 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  $K_a$ ,  $K_b$ ; OH the pH scale, the pOH,  $pK_w$ ,  $pK_a$ ,  $pK_b$ , etc., numerical problems, aqueous solutions of salts – hydrolysis 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.
- B. Solid – solution equilibrium, the 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.
- C. Oxidation and Reduction, redox and distribution – (in two phases) equilibria; redox equilibrium and ion–electron method of balancing redox equations, disproportionation relations.

Chemistry in Non-aqueous solvents (Common nonaqueous 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  $SO_2$ ).

Molecular structure and bonding: Fajan'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), Wades rule, Boron nitrides (structure and bonding), Silicate chemistry (Structure and bonding), Silicone (structure and bonding), Phosphazene, interhalogen compounds, polyhalide ions, pseudohalogens Bonding of

noble gas compounds, Defects in solids. Stoichiometric defect: Schottky and Frenkel defects, Non-stoichiometric imbalance in crystals (outline). Band theory: band gap, metals, insulators, semiconductors (intrinsic and extrinsic), Crown ether complexes of alkali metals.

### **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.

*Prerequisites:* Chemical Principles (CHY111).

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

This course is designed 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**

**Thermodynamics & Thermochemistry:** First, second and third laws of thermodynamics and their applications in chemistry, Enthalpy change and its impact on material science and biology, Enthalpies of formation and reaction enthalpies, Internal energy, entropy, Gibbs free energy, Ideal Gas Law, Kinetic Theory of Gases, Maxwell-Boltzmann Distribution

**Entropy and Information:** Absolute temperature, Shannon Entropy

**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

**Acid-base equilibria:** Open systems

**Chemical Kinetics:** Determination of rate, order and rate laws, Impact of Chemical Kinetics on Biochemistry:

**Catalysis** (Activation energy, Arrhenius equation), **Diffusion across membranes** (Osmosis and reverse osmosis), Adsorption and Chromatography, Ion Exchange columns and water purification

**Electrochemistry:** Electrochemical cell notation, half-reaction and electrodes, Varieties of cells, cell potential at equilibrium and non-equilibrium conditions, Standard electrode potentials, Nernst Equilibrium Potential, Voltage-gated ion channels

**Protein-ligand binding:** Binding free energy, Force fields, Empirical potentials, Conformational freedom

**Statistical Thermodynamics:** Microcanonical, Canonical and Grand Canonical Ensembles, Partition function

**Molecular Reaction Dynamics:** Transition State and Potential Energy Surfaces, Effect of translational and vibrational kinetic energy.

## Lab Schedule:

Exp No.	Exp. Name
1	Safety rules/quiz Download Vernier 3.8 for next week
2	Determine $K_{eq}$ for $(KSCN) + Fe(NO_3)_3$
3	Determination of Enthalpy (Bleach – Acetone)
4	Determination of equilibrium constant for Bromocresol Green
5	Acid Rain experiment
6	Arrhenius equation using $KMnO_4$ – Oxalic Acid
7	TLC Analysis of Analgesic Drugs
8	Photosynthesis
9	Order of reaction with respect to Crystal Violet ( $Crystal\ Violet-OH^+$ )
10	Order of reaction with respect to $OH^-$ ( $Crystal\ Violet-OH^-$ )
11	$Crystal\ Violet-OH^+$ (Arrhenius)

*Prerequisites:* Chemical Principles (CHY111).

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

#### Course Content

- Introduction: Importance of Group Theory in Chemistry
- Symmetry elements and symmetry operations: Use molecular models to identify symmetry elements of different molecules. Understanding of the interrelation of different symmetry elements present in a molecule, product of symmetry operations.
- Point Groups: Concepts and properties of a group, group multiplication Tables, Similarity transformation, Class, Determination of symmetry point group of molecules.
- Matrix representations and Character Tables: Matrix representation of groups, reducible and irreducible representations, Great orthogonality theorem, character tables.
- Direct product, Molecular vibrations: Direct Product and Spectroscopic selection rule, Molecular Vibrations, Normal coordinates, Symmetry of normal mode vibrations, Infrared and Raman active vibrations. Hückel MO theory.

*Prerequisites:* Chemical Principles (CHY111); Mathematical Methods I (MAT103).

### ❖ **CHY214: Physical Methods in Chemistry** (3 credits: 2 Lectures + 0 Tutorial + 1 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<sub>2</sub>.
- 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:**

- A. **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.

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

**Lab Schedule:**

Expt No.	Experiment Name
<b>Unit-1</b>	
1	Introduction to UV-vis/photoluminescence/NMR and Grading scheme/Safety Rules
2	Characterization of various solvents by UV-vis technique - Displaying Data Graphically
3	Characterization of various organic dyes by UV-vis technique- Displaying Data Graphically
4	Characterization of various organic luminescence dyes by photoluminescence spectrometer- Displaying Data Graphically
5	Characterization of various organic molecules by NMR technique- Displaying Data Graphically
6	Determination of molecular mass of organic compounds
<b>Unit-2</b>	
7	IR: Determination of Functional Groups
8	IR: Determination of Functional Groups
9	Identification of stretching, bending and combination bands of water
10	Study of isotope effect using IR spectroscopy
11	TLC/HPLC Experiment: Working principle and demonstration
12	TLC/HPLC Experiment: Separation of small molecules
<b>Unit-3</b>	
13	Sample preparation and crystallization (Small molecule)
14	Small molecule crystal selection, data collection
15	Small molecule structure determination
16	Sample preparation and Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA) experiments (small molecule)
17	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 Substitution ( $S_N1$ ,  $S_N2$ ,  $S_N1'$ ,  $S_N2'$ ,  $S_{Ni}$ ) 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 utility.

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	E1. Melting point determination of recrystallized sample, TLC of samples
3	E2. Nucleophilic substitution reaction.
4	E4. Factors that affect the relative rate of the $S_N2$ reaction.
5	E5. Factors that affect the relative rate of the $S_N1$ reaction.
6	E6. Oxidation of benzaldehyde to benzoic acid.
7	E7. Borohydride reduction of a ketone: hydrobenzoin from benzil.
9	E8. Benzoylation of a given compound
10	E9. Halogenation of acetanilide/benzanilide
11	E10. Bromination of stilbene
12	E11. Synthesis of dye
13	Viva

*Prerequisites:* Basic Organic Chemistry-I (CHY122).

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

### 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  $\beta$ -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:** oxidation of carbonyls -Jones oxidation, Oppenauer oxidation, functional group interconversion through oxidation; reduction of carbonyls:  $\text{NaBH}_4/\text{LiAlH}_4/\text{diborane}$  reduction, Cannizzaro 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	E0. Introduction to the lab notebook requirements and grading
2	E1. Osazone reaction: Identification of an unknown Sugar (addition reaction)
3	E2. Preparation of Dibenzylideneacetone (Aldol condensation)
4	E3. Synthesis of Isopentyl acetate (Esterification)
5	E4. Benzilic acid from Benzil (Rearrangement reaction)
6	E5. Synthesis of the Commercial Antidepressant Moclobemide (Amide bond formation)
7	E6. Preparation of Benzopinacol from benzophenone (Reduction by Zn metal)
8	E7a. Preparation of Benzyl alcohol from Benzaldehyde (Cannizzaro Reaction)
9	E7b. Preparation of Benzoic acid from Benzaldehyde (Cannizzaro Reaction)
10	E8. Estimation of Vitamin C (Iodometric method)
11	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

- General discussion about oxidation and reduction, electron transfer vs atom transfer, oxidation no.
- Concept of electrochemistry, Definition: 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.
- 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

Metals ions play important role in producing color in so called "coordination complexes". Understanding of the coordination complexes lies at the heart of coordination chemistry. 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 color 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, linkage isomerism, electronic effects, steric effects, geometry, Fluxional molecule.

- **Chelate and Macrocyclic 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<sub>2</sub>, N<sub>2</sub>, CN<sup>-</sup>, H<sub>2</sub>O, NH<sub>3</sub>, BF<sub>3</sub> 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 includes Orgel diagrams (qualitative approach), hole formalism – inversion and equivalence relations, selection rule for spectral transitions, d-d spectra and crystal field parameters, nephelauxetic series. Spinels.
- **Magnetism:** Meaning of magnetism, diamagnetic, paramagnetic, ferromagnetic materials, and magnetic measurement.

#### Lab Schedule:

Exp. No.	Experiment Name
1	Preparation and UV-Visible spectroscopic study of simple coordination complexes, such as hexaaquacobalt(II), hexaaquacopper(II), hexaaquanickel(II) ions.
2	Synthesis of [Ni(disalicylaldehyde-1,2-phenylenediamine)] coordination complex
3	Characterization of [Ni(disalicylaldehyde-1,2-phenylenediamine)] coordination complex using IR, UV-vis, NMR
4	Analysis of [Ni(disalicylaldehyde-1,2-phenylenediamine)] coordination complex
5	Synthesis of [VO(2,4-pentanedione) <sub>2</sub> ]
6	Characterization of [VO(2,4-pentanedione) <sub>2</sub> ] by using IR, UV-vis, NMR
7	Analysis of [VO(2,4-pentanedione) <sub>2</sub> ]
8	Study of solvatochromic property of [VO(2,4-pentanedione) <sub>2</sub> ]
9	Synthesis of [Cr(2,4-pentanedione) <sub>3</sub> ]
10	Characterization of [Cr(2,4-pentanedione) <sub>3</sub> ] by using IR, UV-vis, NMR
11	Analysis of [Cr(2,4-pentanedione) <sub>3</sub> ]
12	Synthesis of [Co(2,4-pentanedione) <sub>3</sub> ]
13	Characterization of [Co(2,4-pentanedione) <sub>3</sub> ] by using IR, UV-vis, NMR
14	Analysis of [Co(2,4-pentanedione) <sub>3</sub> ]

*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 advance part of the electrochemistry and chemistry of s and p block elements.

### Course content:

- Electromotive Force: Factors affecting the EMF of half cells: (i) effect of concentration; (ii) effect of pH (iii) effect of precipitation and (iv) effect of complex formation; Periodic trends in reduction potential; Latimer diagram vs. Frost diagram; Titration based on redox potential; Redox indicators; Potentiometric titrations (acid-base, redox, precipitation)
- Electrode potential measurement: 3 electrode system: working electrode, reference electrode and counter electrode; comparison between three and two electrode system; Linear sweep voltammetry, Cyclic voltammetry (CV), Differential pulse voltammetry (DPV) etc.; Why pulse voltammetry is more accurate? Bulk electrolysis, Electrode kinetics-heterogeneous electron transfer
- Water oxidation and reduction, effect of pH;
- Chemistry of s and p Block Elements: Relative stability of different oxidation states, diagonal relationship and anomalous behavior of first member of each group. Allotropy and catenation. Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate: study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Beryllium hydrides and halides.
- Chemistry of Al, Ga, In, Ge, Sn, Pb, As, Sb, Bi, Se, Te.
- Trans effect, Inner sphere and outer sphere electron transfer.
- Complex Equilibria: Thermodynamic and stoichiometric stability constants of metal-ligand complexes. Complexometric titration with EDTA; Determination of composition and stability constants of complexes by pH-metric, spectrophotometric and polarographic methods.

### Lab Schedule:

Exp. No.	Experiment Name
1	Determination of a mixture of carbonate and hydroxide by using double indicator method
2	Analysis of mixture of carbonate and bicarbonate
3	Titration with $\text{KMnO}_4$ a. Standardization of $\text{KMnO}_4$ solution with standard oxalic acid solution. b. Estimation of Fe(II) using standardized $\text{KMnO}_4$ solution. c. Estimation of Fe(III) and Mn(II) in a mixture using standardized $\text{KMnO}_4$ solution.
4	Titration with $\text{K}_2\text{Cr}_2\text{O}_7$ a. Estimation of Fe(II) using $\text{K}_2\text{Cr}_2\text{O}_7$ solution. b. Estimation of Fe(III) using $\text{K}_2\text{Cr}_2\text{O}_7$ solution. c. Estimation of Fe(II) and Fe(III) in a given mixture using $\text{K}_2\text{Cr}_2\text{O}_7$ solution. d. Estimation of Fe(III) and Cu(II) in a mixture using $\text{K}_2\text{Cr}_2\text{O}_7$ .
5	Complexometric titration a. Zn(II) and Cu(II) mixture.
6	Gravimetry analysis a. Estimation of Ni(II) using Dimethylglyoxime (DMG). b. Estimation of Al(III) by precipitating with oxine and weighing as $\text{Al}(\text{oxine})_3$ .
7	VIVA

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

❖ **CHY311: Chemical Binding** (4 credits: 3 Lectures + 0 Tutorial + 3 h Computer Lab) Monsoon

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

**Course content**

- Theorems of Linear Algebra
- Postulates of Quantum Mechanics
- Atomic Orbitals and Basis Sets
- Born-Oppenheimer approximation and the molecular Hamiltonian
- The Concept of the Potential Energy Surface
- Geometry Optimization and Frequency Analysis
- Semi-empirical and *ab initio* Quantum Mechanics
- Variation and Perturbation Theory
- Spin, statistics and the Pauli principle
- Valence Bond and Molecular Orbital theories
- Independent-Particle Models: the Hartree method
- The Hartree-Fock Self-Consistent Field equations
- Electron Correlation, Density Matrices and Natural Orbitals
- Density Functional Theory
- Atoms in Molecules
- Periodic systems
- Implicit and explicit solvent methods

*Prerequisites:* Chemical Principles (CHY111), Physics (PHY101/PHY103/PHY102/PHY104), and Mathematical methods (MAT101/ MAT103)

*Co-requisite:* Molecular Spectroscopy (CHY313).

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

In this course, Rotational, Vibrational, UV-Visible, Fluorescence, Mass 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.

Mass spectrometry: Introduction to mass spectrometry, mass spectrometer, isotope effect, Chemical ionization, Electron impact ionization, fragmentation patterns. Applications.

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: Grignard Reaction, Aldol Condensation, Diels Alder Reaction, Ring Closing Metathesis, Heck Reaction, Negishi Reaction, Suzuki Reaction, Benzoin condensation, Reformatsky reaction, Ugi reaction, Wittig 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, Hetero Diels Alder reaction, Click reaction.

C-O Bond forming reactions and Mechanism: Allan-Robinson Reaction, Baeyer-Villiger Reaction, Fisher Oxazole synthesis, Ferrier Reaction, Glycosidation reaction, Sharpless asymmetric Epoxidation.

Oxidation, Reduction reactions and Mechanism: Bayer-Villiger oxidation, Dess-Martin periodinane oxidation, Swern Oxidation, Corey–Kim oxidation, Jones Oxidation, Luche reduction, Birch reduction, Gribble reduction.

Rearrangement Reactions and Mechanism: Benzilbenzilic acid rearrangement, Pinacol Pinacolone rearrangement, Fries rearrangement, Amadori rearrangement, Beckmann rearrangement, Demzanov rearrangement, Payne rearrangement, Wallach rearrangement, Ferrier rearrangement

Conjugate addition reactions and Mechanism: 1,2-addition reaction, 1,4-addition reaction, Reformatsky reaction, Prins reaction, Michael 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 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

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

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

This course aims at helping the student to understand the concept of organometallic and basic bioinorganic chemistry. In first half we will cover organometallic chemistry and after taking this course student can able to differentiate coordination chemistry and organometallic chemistry. In second half of the course, we will cover some example of organometallic catalyst, basic bioinorganic chemistry and mechanistic understanding of metals in biological reactions.

#### **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 cyanides; Linear nitrosyl vs bent nitrosyls.
- Phosphine as spectator ligands.
- Alkene and alkyne as ligand; Structure and bonding of Ziegler-Natta salt, Bonding in terms of molecular orbital.
- Carbene chemistry: Fischer vs Schrock carbene, Stability and reactivity of singlet and triplet carbene (e.g.  $\text{Li}_2\text{C}$  vs  $\text{H}_2\text{C}$  vs  $\text{F}_2\text{C}$  etc.); Synthesis and application; N-heterocyclic Carbene, Carbene vs carbenoid (introductory level); Zero-electron ligand, delta bonding.
- Alkyl, aryl and ligands with higher hapticity: Hapticity; MO approach; Cyclic and acyclic polyenyl pi-bonded ligands; Sandwich compounds; Chemistry of  $\text{Cp}^*$ ; 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.
- Outline of C-C coupling reactions.
- Catalysis: Heterogeneous catalysis; Terminology in catalysis, Application of chiral phosphine ligand in catalysis.
- Organometallic chemistry of p-block elements.
- Metals in biology; Iron storage and transport, Na-K pump.
- Oxygen transfer protein: Hemoglobin, Myoglobin, Hemocyanin and Hemerythrin. Outline of Fe-based enzyme.
- Nitrogen fixation: Nitrogenase
- The Zn<sup>2+</sup> ion: Nature's Lewis acid
- Cu protein
- OEC complex

*Prerequisites:* Coordination Chemistry (CHY242).

❖ **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)

❖ **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 Chemistry
  - 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 and synthetic polymers such as carbohydrates, nucleic acids, proteins and polymers. The chemistry and biochemistry associated with these macromolecules will be discussed with examples. The goal is to learn about these important natural and synthetic 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 and Polymers

**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, 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 i.e. Nucleic acids, 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), RNA (Basic structure and functions), DNA Transcription and DNA translation, Summary of Nucleic acid

**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  $\text{Cu}^{+2}$  ions, Ninhydrin test, Post translational modifications (phosphorylation, glycosylation etc.), Preparation of amino acids, Strecker synthesis, Gabriels phthalimide synthesis

Protein Structure and quick overview of primary, secondary, tertiary and quaternary structure, Structure determination of peptides 4.12.1. N-terminal analysis by Edmann degradation, C-terminal (thiohydantoin and carboxypeptidase), Synthesis of simple dipeptides by N-protection (t-butoxycarbonyl and phthaloyl), C-activating group and Merrifield solid phase synthesis, Thermodynamics and Kinetics of Proteins, Protein Evolution, Summary of Proteins

**Polymers:** Basic concepts in Polymer Chemistry, Nomenclature, Classification, Structure and properties of Polymers, Natural Occurring Polymers/synthetic polymers, Polymer synthesis, Step-growth polymerization, Chain Growth Polymerization, Free Radical, Ionic (Cationic and Anionic)

Molecular weight determination (Number average and weight average MW, Measurement of Number average MW), Polymer morphology, Amorphous state and rheology, Glass transition temperature, Crystallinity, Liquid crystallinity,

Polymer properties (Structure property correlation), Mechanical Properties, Thermal Stability, Polymer degradation, Chemical resistance, Molecular weight and intermolecular forces, Physical and chemical crosslinking, Non-linear optical properties (in brief), Applications of polymers

*Prerequisites:* Basic Organic Chemistry-II (CHY221)

❖ **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  $\pi$  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).

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

The aim of the course is advance level of Bio-inorganic Chemistry.

#### Course content:

- i. General discussion about bioinorganic chemistry
- ii. Biological important elements, Biological ligands
- iii. 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

iv. Importance of Oxygen, Great oxygenation event

v. Iron based chemistry in nature; Iron metabolism: Iron transport, Iron storage; Iron cycle.

vi. Oxygen utilization: (i) Oxygen transport and storage (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.

vii. Fe-S protein, Hydrogenase enzyme.

viii. Toxicity: Superoxide dismutase and Catalase

ix. Mo-containing enzyme: Nitrogenase, nitrogen cycle.

x. Co, V containing enzymes.

xi. Zn containing enzymes.

xii. Photosynthesis: O-H bond activation, role of Mn in OEC

*Prerequisites:* Coordination Chemistry (CHY242) or 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, Krebs'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<sup>+</sup>-NADPH, Biosynthesis of Niacin (Vitamin B3), FAD-FADH-FADH<sub>2</sub>, 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)

❖ **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)

❖ **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 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 modern materials such as semi-conductors (organic, inorganic) and novel nanostructures.

### **Course content**

Introduction, Bulk Vs. Nano, Quantum confinement effect, Surface area to volume ratio, Effects on the Properties of Semiconducting and Metallic Materials (electrical, magnetic, mechanical etc.) and structural properties, Carbon nano-architectures: Fullerene, SWNT, MWNT, Graphite etc., Classification of structures, nanoparticles and Q-Dots, 2D materials, nanowires and their properties, Bonding, Methods of preparation, Nanomaterial's synthesis: Top down and Bottom up approach, Physical and chemical methods, Applications (in brief Nano-machines, solar cells, coatings, MEMS, nano-medicine, sensors, miscellaneous) Characterization Techniques and Instruments: Microscopy SEM, TEM, AFM, X-Ray diffraction, UV-vis, Photoluminescence, Raman, FTIR, ESR, XPS, BET, DLS, Zeta potential

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

**B.Sc. (Research) Chemistry & Minor in Chemistry**  
Recommended Semester-wise Plan

Semester	Course	Course Title	L:T:P	Minor	Prerequisites	Credits	
						Major	Minor
<b>1</b> (MSN)	CHY111	Chemical Principles	3:1:1	□	None	5+12	5
	PHY101/ PHY103	Introduction to Physics-I/ Fundamentals of Physics-I	3:1:1		None		
	MAT103	Mathematical Methods-I	3:1:0		None		
	BIO201*	Cell biology and Genetics*	2:0:1		PCB at 10+2		
<b>2</b> (SPR)	CHY114	Molecular modelling <sup>#</sup>	1:0:1		None	12+5	7
	CHY144	Inorganic Chemistry-I	3:0:0	□	CHY111		
	CHY122	Basic Organic Chemistry-I	2:1:1	□	CHY111		
	CHY214	Physical Methods in Chemistry <sup>#</sup>	2:0:1		CHY111		
	PHY102/ PHY104	Introduction to Physics-II/ Fundamentals of Physics-II	3:1:1		None		
	BIO113*	Essentials of Biology*	2:0:1		non-PCB at 10+2		
<b>3</b> (MSN)	CHY211	Chemical Equilibrium	3:1:1	□	CHY111	15	9
	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		
<b>4</b> (SPR)	CHY212	Chemical Applications of Group Theory	3:0:0		CHY111, MAT103	11+4	
	CHY222	Chemistry of Carbonyl Compounds	2:1:1		CHY122, CHY221		
	CHY242	Coordination Chemistry	3:0:1		CHY111, CHY122, CHY144		
	MAT084	Basic Probability & Statistics	3:1:0		None		
<b>5</b> (MSN)	CHY311	Chemical Binding	3:0:1		CHY111, PHY101/103/102/104, MAT101/103; CHY313	16	
	CHY313	Molecular Spectroscopy	3:1:0		CHY111, CHY214		
	CHY 321	Named Organic Reactions and Mechanism	2:0:0		CHY221		
	CHY323	Organometallic and Bio-inorganic Chemistry	3:0:0		CHY242		
	CHY351	Macromolecules	3:0:0		CHY221		
<b>6</b> (SPR)	CHY322	Heterocyclic Chemistry	3:0:0		CHY221, CHY321	9+3	
	CHY342	Chemistry of Solids and Surfaces	3:0:0		CHY111, CHY214 or PHY101/102/103/104		
	CHY332	Informatics & Machine Learning	2:0:1		CHY111, MAT284/MAT084, CHY114/BIO101/MAT110/PHY105/CSD101		
	CHYxxx	Electives	3:0:0		†		
<b>7</b> (SPR)	CHY498	Senior Project	0:0:6			6+3	3
	CHYxxx	Electives	3:0:0	□	†		
<b>8</b> (SPR)	CHY499	Senior Project	0:0:6			6+3	
	CHYxxx	Electives	3:0:0		†		
Graduation	<b>Total Credits</b>			<b>24</b>		<b>110</b>	<b>24</b>

\*BIO113/BIO201: any one course

<sup>#</sup> 2h lab

† specific to course

## Future courses

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

#### Course content

- General Principles 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 be 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, Chemical Binding, Macromolecules.

### ❖ **CHY413: Applications of analytical techniques** (3 credits: 3 Lectures)

Applications of UV, IR, NMR, and mass spectral methods in structure elucidation /determination of organic compounds.

*Pre-requisites:* Physical Methods in Chemistry (CHY214), Molecular spectroscopy (CHY313)

### ❖ **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)

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

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.

*Prerequisites:* Basic Organic Chemistry-II (CHY221) or Macromolecules (CHY351).

❖ **CHY456: Food Chemistry** (3 credits: 2 Lectures + 1 Lab)

The course provide basic scientific principles to food systems and practical applications. How quality of food is related to the chemical and biochemical reactions of carbohydrates, lipids, proteins, and other constituents in fresh and processed foods. An emphasis of reaction and processing conditions and its effect on color, flavor, texture, nutrition value, and safety of food will be discussed. Real world problems associated with the food industry and lab experiments to reinforce class discussions will be there. Activation and control of enzymatic reactions in fruits and vegetables; consequences of water migration on food quality; gelatinization-retrogradation in starch-based foods (e.g., pudding, bread, and rice); initiation and control of non-enzymatic browning (e.g., meat); food emulsions (e.g., salad dressings, commutated meats products), pickles and sauces; sugar vs sweet a healthy mode, flavoring agents, mode of cooking will be discussed.

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

❖ **CHY 542: Frontiers in Inorganic Chemistry** (3 credits: 3 Lectures + 0 Tutorial + 0 Lab)

In this course we will explain the advances in inorganic chemistry and student will learn concept of physical inorganic chemistry using molecular orbital approach, spectroscopy and reaction kinetics.

Course Content:

1. Metal-centered electronic spectra of transition metal complexes: microstates, determination of ground and all excited state terms of  $d^n$  ions, splitting of  $d^n$  terms in octahedral and tetrahedral fields, Qualitative idea of Tanabe-sugano diagrams, Charge transfer spectra according to MO theory. Magnetic properties of coordination compounds: spin and orbital moment, spin-orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable-temperature magnetic moments.
2. Inorganic Reaction Mechanism: Mechanism of substitution reactions, : solvent exchange, aquation, anation, base hydrolysis, acid catalysed aquation, pseudo-substitution. Four broad classes of mechanism of substitution – ‘D’, ‘A’, ‘Ia’ and ‘Id’. Mechanism of isomerization reaction – linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemization, Ray-Dutta and Bailar twist mechanisms. Inner and outer sphere electron transfer. Proton coupled electron transfer (PCET)
3. Inorganic rings, cages and clusters: Wade’s rules, Carboranes, Metalloboranes. Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, capping rules, carbide, nitride, chalcogenide and halide containing clusters. Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis. Iso- and heteropolyoxometalates with respect of V, Mo and W: syntheses, reactions, structures, uses. Metal-metal bonding (M.O. concept), metal-metal bonded dinuclear d-metal complexes-typical examples. Bonding in dirhenium complexes.
4. 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.
5. 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.

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

*Co-requisites:* Organometallic and Bio-inorganic Chemistry (CHY323)