# M.Sc. (5-Year Int.)
# 2020 and 2021 Batches

### School of Chemistry

**(Based on UGC – Learning Outcomes-Based Curriculum Framework)**

**Vision Statement:**

To be the source of knowledge and center of training that imparts a sound foundation in chemical sciences with strong transdisciplinary reach, and spawns original and innovative research in contemporary and futuristic chemical themes.

**Mission Statements:**

- Providing quality chemical sciences education at masters and doctoral levels
- Conducting fundamental and advanced research in chemical sciences
- Establishing research collaborations with other universities/institutes/laboratories
- Carrying out sponsored research and development projects from international/national government and private partners

## Qualification Descriptors (QDs)

Utilizing basic knowledge and laboratory skills gained in chemical and allied sciences to:

QD-1 analyze, interpret and explain chemically and related relevant observations

QD-2 identify critical scientific issues and provide potential resolutions

QD-3 create/cultivate new generations of human resource in chemical and allied sciences

QD-4 formulate innovative and relevant scientific problems and develop solutions

## Mapping Qualification Descriptors (QDs) with Mission Statements (MS)

| | MS-1 | MS-2 | MS-3 | MS-4 |
|---|---|---|---|---|
| **QD-1** | 3 | 3 | 1 | 1 |
| **QD-2** | 3 | 3 | 1 | 1 |
| **QD-3** | 3 | 3 | 2 | 1 |
| **QD-4** | 3 | 3 | 3 | 3 |

## Program Learning Outcomes (PLOs)

After going through the five years of study, chemistry graduates can use the comprehensive knowledge and skills gained, to:

PLO-1: observe, analyze and interpret scientific phenomena and process

PLO-2: design and develop new molecules/processes with industrial and societal applications

PLO-3: formulate new ideas/concepts in chemical and allied sciences and test them

PLO-4: communicate effectively the principles and practice of science, chemistry in particular

PLO-5: address issues of environment, health and development from a chemical perspective

PLO-6: follow professional ethics in all spheres of activity

PLO-7: function effectively as a member/leader in diverse teams/groups

PLO-8: engage in independent learning in the broadest context of scientific advancement

## Mapping of Program Learning Outcomes (PLOs) with Qualification Descriptors (QDs)

| | QD-1 | QD-2 | QD-3 | QD-4 |
|---|---|---|---|---|
| **PLO-1** | **3** | **3** | **2** | **2** |
| **PLO-2** | **3** | **3** | **2** | **3** |
| **PLO-3** | **3** | **3** | **2** | **3** |
| **PLO-4** | **2** | **2** | **3** | **2** |
| **PLO-5** | **2** | **2** | **3** | **3** |
| **PLO-6** | **1** | **1** | **3** | **2** |
| **PLO-7** | **3** | **3** | **3** | **3** |
| **PLO-8** | **3** | **3** | **3** | **3** |

# Course Structure

## I Year

### I Semester (*23 credits*)

| Number | Title | Credit |
|---|---|---|
| MA101 | Mathematics I | 4 |
| PH101 | Mechanics | 4 |
| CY101 | Stoichiometry, solutions and gases | 3 |
| SB101 | Environmental studies | 3 |
| PH102 | Mechanics lab | 1.5 |
| CY102 | Qualitative analysis | 1.5 |
| | Biology lab | 1.5 |
| | IT lab | 1.5 |
| | English | 3 |

### II Semester (*19 credits*)

| Number | Title | Credit |
|---|---|---|
| MA151 | Mathematics II | 4 |
| PH151 | Waves, oscillations, sound and light | 3 |
| CY151 | Energetics and kinetics | 3 |
| SB151 | Introductory biology | 3 |
| PH152 | Waves and oscillations, sound and light lab | 1.5 |
| CY152 | Quantitative analysis | 1.5 |
| | Introductory biology lab II | 1.5 |
| | IT lab II | 1.5 |

## II Year

### III Semester (*18.5 credits*)

| Number | Title | Credit |
|---|---|---|
| MA201 | Mathematics III | 4 |
| PH201 | Electricity and magnetism | 4 |
| CY201 | Structural chemistry | 3 |
| SB201 | Molecules, genes and information processing | 3 |
| PH202 | Electricity and magnetism lab | 1.5 |
| CY202 | Physical chemistry lab | 1.5 |
| | Molecules and information processing lab | 1.5 |

### IV Semester (*21.5 credits*)

| Number | Title | Credit |
|---|---|---|
| MA251 | Mathematics IV | 3 |
| PH251 | Modern physics | 4 |
| CY251 | Basic organic chemistry | 3 |
| SB251 | Structure and function of macromolecules | 3 |
| PH252 | Physics lab IV | 1.5 |
| CY252 | Identification of organic compounds lab | 1.5 |
| | Biology lab IV | 1.5 |
| | *Electives for **4 credits** from:* | 4 |
| CY253 | Introductory supramolecular chemistry | 2 |
| CY254 | Elementary polymer chemistry | 2 |
| | Any other physics/maths/biology course | |

## III Year

### V Semester (*19 credits*)

| Number | Title | Credit |
|---|---|---|
| CY301 | Inorganic chemistry | 3 |
| CY302 | Organic chemistry: Synthesis and reactions | 3 |
| CY303 | Analytical chemistry | 3 |
| CY304 | Surface and electrochemistry | 3 |
| CY305 | Organic chemistry: Conformation and reactivity | 3 |
| CY306 | Organic chemistry lab | 2 |
| CY307 | Analytical chemistry lab | 2 |

### VI Semester (*18 credits*)

| Number | Title | Credit |
|---|---|---|
| CY351 | Instrumental methods of analysis | 3 |
| CY352 | Industrial and environmental chemistry | 3 |
| CY353 | Organic rearrangements and natural products | 3 |
| CY354 | Computer programming and numerical methods | 3 |
| CY355 | Inorganic chemistry lab | 2 |
| CY356 | Industrial chemistry lab | 2 |
| CY357 | Open-ended lab | 2 |

## IV Year

### VII Semester (*18 credits*)

| Number | Title | Credit |
|---|---|---|
| CY401 | Basic concepts and coordination chemistry | 3 |
| CY402 | Physical organic chemistry | 3 |
| CY403 | Quantum chemistry | 3 |
| CY404 | Symmetry, Group Theory and Mathematics | 3 |
| CY405 | Inorganic chemistry lab: Quantitative and qualitative analysis | 3 |
| CY406 | Advanced Organic chemistry Lab | 3 |

### VIII Semester (*21 credits*)

| Number | Title | Credit |
|---|---|---|
| CY451 | Main group and inner transition elements | 3 |
| CY452 | Organic reactions and mechanisms | 3 |
| CY453 | Molecular spectroscopy | 3 |
| CY454 | Chemical and statistical thermodynamics | 3 |
| CY455 | Biological chemistry | 3 |
| CY456 | Inorganic chemistry lab: Synthesis | 3 |
| CY457 | Physical chemistry lab | 3 |

## V Year

### IX Semester (*21 credits*)

| Number | Title | Credit |
|---|---|---|
| CY501 | Spectroscopic methods for structure elucidation | 3 |
| CY502 | Advanced organic synthesis | 3 |
| CY503 | Project - I | 3 |
| CY504 | Chemical dynamics | 3 |
| CY505 | Chemical binding | 3 |
| CY506 | Advanced inorganic chemistry | 3 |
| CY507 | Computer Applications and Programing Lab | 3 |

### X Semester (*20 credits*)

| Number | Title | Credit |
|---|---|---|
| CY551 | Chemistry of materials | 3 |
| CY552 | Project - II | 9 |
| CY571 to CY586 | Electives for ***8 credits*** from: (See titles in the Syllabus) | 8 |

**Course Code : CY101**
**Title of the Course : Stoichiometry, Solutions and Gases**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** Basic chemistry course

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1:** understand the basic atomic structure, subatomic particles involved and nomenclature of the binary ionic, molecular compounds.

**CLO-2:** understand the basic stoichiometric calculations involved in the chemical reactions and balancing the equations.

**CLO-3:** understanding the solution chemistry involving the colligative properties and redox reactions. To explain the ideal and non-ideal behavior of solutions.

**CLO-4:** apply the basic concepts of gas laws in various applications in day to day life.

**CLO-5:** understanding the basic concepts of colloids and its application in the commercially viable technologies.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| CLO-1 | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| CLO-2 | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| CLO-3 | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| CLO-4 | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| CLO-5 | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus – CY101

Experimental evidence for the atomic hypothesis. Chemical compounds and their composition - introduction to nomenclature.

Chemical reactions and stoichiometric calculations.

Solution chemistry - electrolytes and non-electrolytes. Colligative properties. Ideal and non-ideal solutions. Reactions in solution - redox, acid-base, precipitation, ion exchange.

Colloids. Properties of gases - Avogadro's hypothesis, the ideal gas law. Kinetic molecular theory.

Gas mixtures. Solubility of gases. Gases at high pressure and low temperatures - critical phenomena.

**Reference Books:**

- Chemistry by McMurry and Fay
- Physical Chemistry by Peter Atkins and Julio de Paula
- Physical Chemistry by Gilbert Castellan
- Physical Chemistry by Robert G. Mortimer

**Course Code : CY102**
**Title of the Course : Qualitative Analysis Lab**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 1.5

**Prerequisite Course / Knowledge (If any):** A course on chemistry at higher secondary school level

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basic concepts of experiments in chemistry

**CLO-2 :** safely handle of chemicals and glass apparatus and in a chemistry lab

**CLO-3 :** perform chemical reactions in test tubes

**CLO-4 :** develop observation skills and interpretation of observations

**CLO-5 :** identifya few elements in a substance

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 2 | 2 | 1 | 1 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 1 |
| **CLO-3** | 1 | 2 | 3 | 3 | 3 | 3 | 2 | 2 |
| **CLO-4** | 1 | 2 | 2 | 2 | 3 | 3 | 3 | 2 |
| **CLO-5** | 1 | 1 | 1 | 2 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY102)

Observation of reactions of common cations and anions.
Semimicro analysis of mixtures and Group separation of cations

Following radicals (anions and cations) analysis will be conducted in this course:

**Anions or Acid radicals:** Nitrate ($NO_3^-$), Sulfate ($SO_2^-$), Nitrite ($NO_2^-$), Chloride ($Cl^-$), Bromide ($Br^-$), Iodide ($I^-$) Acetate ($CH_3COO^-$), Carbonate ($CO_3^{2-}$), Sulphide ($S^{2-}$), Bromate ($BrO_3^-$), Iodate ($IO_3^-$), Phosphate ($PO_4^{3-}$).

**Cation or Basic Radicals:** Silver ($Ag^+$), Lead ($Pb^{2+}$), Copper ($Cu^{2+}$), Cadmium ($Cd^{2+}$), Tin ($Sn^{2+}$), Iron ($Fe^{3+}$), Chromium ($Cr^{3+}$), Cobalt ($Co^{3+}$), Nickel ($Ni^{2+}$), Manganese ($Mn^{2+}$), Zinc ($Zn^{2+}$), Barium ($Ba^{2+}$), Strontium ($Sr^{2+}$), Calcium ($Ca^{2+}$), Sodium ($Na^+$), Potassium ($K^+$), Ammonium ($NH_4^+$).

**Suggested Reading:**


1. Lab manual provided by teacher
2. Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis
3. Advanced Practical Inorganic Chemistry – Gurdeep Raj

**Course Code : CY151**
**Title of the Course : Energetic and Kinetics**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** NONE

**Course Learning Outcomes (CLOs)**

**CLO-1:** understand the basic concept of temperature, pressure, enthalpy entropy, free energy. Evaluate thermodynamic properties of pure substances using PVT equation-of-states.

**CLO-2:** apply first law of thermodynamics to open and closed systems, apply second law of thermodynamics in analyzing efficiency of heat engines, pumps and refrigerators.

**CLO-3:** understand relation between chemical potential of substance with mole fraction in ideal mixtures and activity in real mixtures using experimental observations of Raoult's and Henry's law for mixtures. Apply these concepts to understand effect of solute concentration on colligative properties.

**CLO-4:** understand phase diagrams of pure substances based on phase stability at different pressures and temperatures and predict phase transitions based on thermodynamic changes. Use phase diagrams to predict miscibility in different systems.

**CLO-5:** understand relation between equilibrium constant and standard Gibbs energy of reaction, concept of standard potential and apply to electrochemical cells, use standard potential to predict thermodynamic properties of chemical reactions.

**CLO-6:** understand concept of reaction rate, order of reaction, homogeneous and heterogeneous reactions, analyses effect of thermodynamic variables such as temperature on rate of reaction and use Arrhenius relation to interpret experimental data, effect of catalyst on rate of reaction, mechanism and rate laws for unimolecular and chain reactions.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | **PLO 1** | **PLO 2** | **PLO 3** | **PLO 4** | **PLO 5** | **PLO 6** | **PLO 7** | **PLO 8** |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 2 | 3 | 1 | 3 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 2 | 3 | 3 | 3 |
| **CLO-3** | 3 | 1 | 2 | 3 | 1 | 3 | 3 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 1 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 2 | 3 | 3 | 3 |
| **CLO-6** | 3 | 1 | 3 | 3 | 1 | 3 | 3 | 3 |

**Detailed Syllabus (CY151)**

Thermochemistry - enthalpy and enthalpy change - calorimetry - enthalpies of formation and of reactions.

Entropy and free energy. State functions.

Chemical equilibrium in the gas phase - equilibrium constants and their relation to free energy temperature dependence.

Equilibrium in the aqueous phase - pH, buffers and indicators - complex ions.

Electrochemistry - voltage and free energy - standard potentials Batteries, fuel cells.

Chemical kinetics - reaction rates - effect of concentration and temperatures. Steady state approximation. Reaction mechanism from rate laws.

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Heterogeneous equilibria - adsorption.

Suggested reading: Will be prescribed by the instructor.

**Course Code : CY152**

**Title of the Course : Quantitative Analysis Lab**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 1.5

**Prerequisite Course / Knowledge (If any):** A practical course on quantitative analysis

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of analytical chemistry and analytical tools.

**CLO-2 :** realize different types of analyses including titrimetry, gravimetry and colorimetry.

**CLO-3 :** differentiate redox titration from acid base titration and complexometric titration.

**CLO-4 :** analyze an unknown sample (e.g., an iron containing natural mineral) quantitatively using / applying their knowledge of titimetry, gravimetry, etc.

**CLO-5 :** teach the rural people about hardness of water, more specifically, of why pond water from a particular place does not form foam, when cloths are washed with a soap.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 2 | 3 | 3 | 2 | 3 | 3 |
| **CLO-2** | 3 | 2 | 3 | 3 | 3 | 1 | 2 | 2 |
| **CLO-3** | 2 | 3 | 2 | 2 | 2 | 3 | 3 | 3 |
| **CLO-4** | 3 | 3 | 2 | 3 | 3 | 3 | 2 | 2 |
| **CLO-5** | 2 | 2 | 3 | 3 | 3 | 2 | 3 | 2 |

## Detailed Syllabus (CY152)

Titrimetry - acid-base, redox, complexometry.

Gravimetry - determination of water of hydration, estimation of sulphate, chloride, aluminium, manganese, iron, nickel.

Colorimetry - Beer's law, estimation of a metal ion (eg., manganese).

**Suggested reading:**

Lab manual

**Course Code : CY201**
**Title of the Course : Structural Chemistry**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** None

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand electronic structures in atoms

**CLO-2 :** appreciate bonding and shapes of molecules and their consequence in physical properties.

**CLO-3 :** understand the different intramolecular forces.

**CLO-4 :** correlate structural and stability aspects of molecules.

**CLO-5 :** understand the structural aspects of crystals.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs) and Program Specific Outcomes (PSOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 2 | 3 | 1 | 2 | 1 | 3 |
| **CLO-2** | 3 | 1 | 2 | 2 | 1 | 2 | 2 | 3 |
| **CLO-3** | 3 | 2 | 3 | 3 | 2 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 3 |
| **CLO-5** | 3 | 3 | 2 | 2 | 1 | 2 | 1 | 3 |

## Detailed Syllabus (CY201)

Electrons in atoms - the orbital concept - shapes and size of atomic orbitals - electron configuration and the periodic table. (4 h)

The chemical bond - ionic and covalent bonding. MO and VB pictures - hybridization, resonance. Bond parameters - energy, polarity, length. (8 h)

Shapes of molecules - VSEPR theory. (4 h)

The hydrogen bond. Intermolecular forces and non-bonded intra-molecular interactions. Molecular conformations. Examples of different structures and their stabilities from tri-atomics to bio-molecules. (6 h)

The solid state - molecular, ionic and metallic crystals. Crystal lattices - unit cells. Common crystal structures. Factors influencing crystal structures in ionic/molecular solids. Allotropes (of carbon and sulphur). Network solids - silicates. (8 h)

X-ray diffraction and elementary treatment of Bragg's law - NaCl and KCl. (6 h)

**Suggested reading :**
Will be prescribed by the instructor.

**Course Code : CY202**
**Title of the Course : Physical Chemistry Laboratory**

**L-T-P** : ~~L / T /~~ P
**Credits** : 0 – 0 – 1.5

**Prerequisite Course / Knowledge (If any):** CY101, CY151, CY152

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** acquire first-hand experience in experimentally measuring several physical quantities.

**CLO-2 :** understand the utility of some of the spectroscopic techniques

**CLO-3 :** learn how conductivity measurements help determination of the end-points of titrations

**CLO-4 :** calculate several thermodynamic properties of different systems

**CLO-5 :** measure various kinetic parameters of the chemical reactions

### Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-2** | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| **CLO-3** | 1 | 2 | 2 | 2 | 2 | 2 | 1 | 1 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-5** | 1 | 2 | 2 | 2 | 2 | 2 | 1 | 1 |

**Detailed Syllabus (CY202)**

1. Molecular weight of a polymer (viscometry)
2. Stoichiometry of a complex (Job's method: colorimetry)
3. Conductometric titrations
4. Heat of solution (calorimetry)
5. Phase diagram of a 2-component system
6. $pK_a$ of amino acid (pH titration)
7. Solubility product
8. Paritition coefficient
9. Rate constant of acid catalysed ester hydrolysis

**Suggested reading:**

1. Physical Chemistry: A Molecular Approach. D. A. McQuarrie and J. D. Simon, University Science books
2. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
3. Physical Chemistry. I. N. Levine, McGraw Hill.
4. Laboratory manual for instructions

**Course Code : CY251**

**Title of the Course : Basic Organic Chemistry**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** None

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand structural features of different organic compounds in terms of stereo and electronic aspects.

**CLO-2 :** appreciate different ways of electron movement in organic reactions through formation of reactive intermediates.

**CLO-3 :** apply curved arrow notation to propose reaction mechanisms.

**CLO-4 :** analyze the stereochemistry of organic compounds.

**CLO-5 :** understand the general reactivity of different common organic functional groups.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 3 | 1 | 1 | 2 | 1 | 3 |
| **CLO-2** | 3 | 1 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 3 |
| **CLO-5** | 3 | 2 | 2 | 1 | 1 | 2 | 1 | 3 |

## Detailed Syllabus (CY251)

**1. Bonding and physical properties of organic molecules (8 h)**

Nomenclature of simple organic compounds (acyclic, cyclic). Concept of hybridization, resonance, orbital pictures of bonding (sp3, sp2, sp, C-C, C-N & C-O system). Inductive effect, bond polarization, and polarizability, steric inhibition of resonance. Hückel's rules for aromaticity & antiaromaticity, homoaromaticity. Physical properties of bond distance, bond angles, mp/bp & dipole moment in terms of structure and bonding. Concept of acids and bases: effect of structure, substituent and solvent on acidity and basicity.

**2. Basic reaction mechanism and intermediates (8 h)**

Mechanism classifications - ionic, radical and pericyclic; heterolytic bond cleavage and heterogenic bond formation, homolytic bond cleavage and homogenic bond formation; representation of mechanistic steps using arrow formalism. Reactive intermediates: carbocation (carbenium and carbonium ions), carbanions, carbon radicals, carbenes-structure using orbital picture, electrophilic/nucleophilic behavior, stability, generation and fate (elementary idea)

**3. Optical activity and stereochemistry (8 h)**

Representation of molecules in saw-horse, Fischer, flying-wedge and Newman formulae and their inter translations, symmetry element and molecular chirality. Configuration: stereogenic unit i) stereocenters: systems involving 1, 2, 3 centers, stereogenicity, chirotopicity, pseudoasymmetric (D/L and R/S) descriptor, threo/ erythro / meso and syn/anti nomenclature. Stereo axis: chiral axis in allenes & biphenyls, R/S descriptor: cis/trans, syn/anti, E/Z descriptors (at C=C and C=N bonds). Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), racemic compounds.

**4. Chemistry of organic functional groups (12 h)**

Alkanes, olefins, alkynes, halides, alcohols, phenols, ketones, aldehydes, carboxylic acids, ethers, derivatives of carboxylic acids, amines, nitro and cyano compounds; synthesis and basic reactivity with mechanisms.

**Suggested Text Books:**

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.

2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.

3. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.

4. I. L. Finar, Organic Chemistry, Vol-1, 6th edition, Pearson Education.

5. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley.

**Course Code : CY252**
**Title of the Course : Identification of Organic Compounds**

**L-T-P** : ~~L / T~~ / P

**Credits** : 0 – 0 – 1.5

**Prerequisite Course / Knowledge (If any):** Chemistry at +2 level

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** learn how to handle organic chemicals, glassware and precautions to be taken for safety in a Chemistry lab

**CLO-2 :** learn to identify specific organic compounds based on functional groups

**CLO-3 :** learn to separate and purify some organic compounds and measure their physical properties

**CLO-4 :** apply the concepts to identify specific organic compounds

**CLO-5 :** apply the concepts to test the purity of organic compounds

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 1 | 3 | 3 | 3 | 1 | 3 |
| **CLO-2** | 3 | 1 | 1 | 3 | 1 | 3 | 1 | 3 |
| **CLO-3** | 3 | 1 | 1 | 3 | 3 | 3 | 1 | 3 |
| **CLO-4** | 3 | 1 | 1 | 3 | 1 | 3 | 3 | 3 |
| **CLO-5** | 3 | 1 | 1 | 3 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY252)

Unit 1: Separation and purification of organic compounds - melting point - boiling point.

Unit 2: Characteristic reactions of functional groups. Identification of unknowns - chemical and spectral methods.

**Reference Books:**

Lab manual

**Course Code : CY253**
**Title of the Course : Introductory Supramolecular Chemistry**

**L-T-P** : L ~~/ T / P~~

**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** Basic chemistry course

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the noncovalent interactions in simple molecules to supramolecules

**CLO-2 :** explain how biological systems rely heavily on supramolecular interactions for structures and functional properties

**CLO-3 :** apply the molecular selectivity principle in host-guest chemistry including neutral, anionic and cationic guests

**CLO-4 :** apply basic concepts of analytical and spectrocospic methods to host-guest chemistry

**CLO-5 :** create a new supramolecules via self-assembly approach

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed syllabus (CY253)

Unit 1: Basic concepts using chemistry examples Intermolecular interactions and hydrogen bonds

Unit 2: Cation binding hosts, cryptands, crown ethers

Unit 3: Anion binding hosts, single and multi-point recognition

Unit 4: Crystal engineering of solid architectures Self-Assembly in nature and materials

Unit 5: Recent examples from literature

**Reference Books:**


1) J. W. Steed & J. L. Atwood (2009), Supramolecular Chemistry, 1st Edition, John Wiley
2) G.R. Desiraju (1989), Crystal Engineering. The Design of Organic Solids, Elsevier
3) G. R. Desiraju, J. J. Vittal, A. Ramanan (1989), Crystal Engineering -A Textbook, World Scientific-IISc Press
4) Recent papers from journals and reviews and monographs, etc

**Course Code : CY254**
**Title of the Course : Elementary Polymer Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** IMSc courses in the I & II semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** Understand the differences between small molecules and macromolecules

**CLO-2 :** Provide insight into the various classes of monomers and polymers

**CLO-3 :** Understand and analyze polymer molecular weights and various physical properties

**CLO-4 :** Apply the basic concept of polymers in designing useful polymer materials

**CLO-5 :** Apply the polymers for advanced applications.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 2 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 2 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY254)

History of macromolecular science. **(1 h)**

Definition of polymer, monomer, repeat unit, polymerization. Classification of Polymers based on source and polymerizations-polymer composition and structure. Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names. Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers) **(5 h)**

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography **(5 h)**

Physical State: Crystalline and Amorphous state, Thermal transitions, Glass-Rubber transition, Mechanical properties- stress-strain behaviour, Elastomer, Fibers and Plastics **(5 h)**

Polymer Synthesis: step, chain and miscellaneous polymerizations, Kinetics of polymerization **(7 h)**

Application of Synthetic Polymers: Materials and Biological importance and uses. **(3 h)**

**Suggested Reading:**

1. Principles of Polymerization by George Odian
2. Introduction to Physical Polymer Science by L. H. Sperling
3. Polymer Chemistry: An Introduction by M. P. Stevens

**Course Code : CY301**
**Title of the Course : Inorganic Chemistry**

**L-T-P** : L ~~/ T / P~~

**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** None

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of nuclear chemistry

**CLO-2 :** understand the basic concepts and roles of acids, bases, buffers and non-aqueous solvents

**CLO-3 :** correlate structure and functions of some key main group elements and their compounds

**CLO-4 :** appreciate structure, nomenclature and properties of transition elements and their complexes

**CLO-5 :** understand organometallic and bioinorganic chemistry

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 3 | 3 | 2 | 1 | 2 |
| **CLO-2** | 3 | 1 | 2 | 3 | 3 | 2 | 1 | 2 |
| **CLO-3** | 3 | 2 | 2 | 3 | 1 | 2 | 1 | 2 |
| **CLO-4** | 3 | 2 | 2 | 3 | 1 | 3 | 1 | 2 |
| **CLO-5** | 3 | 2 | 2 | 3 | 3 | 3 | 1 | 2 |

## Detailed Syllabus (CY301)

**NUCLEAR CHEMISTRY:** **[6 h]**

Origin of the elements - Nuclear stability and nuclear binding energy - Nuclear forces - Nuclear Reactions - Artificial radioactivity - Transmutation of elements - Fission, fusion and spallation - Nuclear energy - Separation and uses of isotopes - Radiochemical methods - Principles of determination of age of rocks and minerals- Radio-carbon dating - Hazards of radiation and safety measures

**ACIDS, BASES AND BUFFERS:** **[3 h]**

Arrhenius, Brönsted-Lowry, and Lewis concepts of acids and bases - Factors affecting strengths of acids and bases - Ka, Kb, Kw, pH etc.- Buffers, Henderson's equation - Hydrolysis of salts - Common ion effect

**NON-AQUEOUS SOLVENTS**: **[3 h]**

Physical properties of a solvent for functioning as an effective reaction medium - Types of solvents and their general characteristics - Reactions in liquid ammonia and liquid sulfur dioxide

**CHEMISTRY OF SELECTED MAIN GROUP ELEMENTS:** **[4 h]**

Hydrogen bonds, Hydrates and water clathrates - Hydrides and dihydrogen - Alkali metal solution in liquid ammonia - Complexation of alkali metal ion by crown ether and cryptands, Alkali metal anions. Diborane – structure and bonding - Noble gas compounds

**COORDINATION COMPOUNDS AND TRANSITION ELEMENTS:** **[14 h]**

Werner's theory – Nomenclature- Chelates- Stereochemistry of coordination numbers 4, 5 and 6 - Various types of isomerism in coordination complexes- Theories of metal-ligand bonding in transition metal complexes – Effective atomic number concept- Valence bond theory of coordination compounds - Limitations of valence bond theory - Crystal-field theory and crystal-field splitting in octahedral and tetrahedral complexes - CFSE and its calculation in different stereochemistries - Weak field and strong field- Low spin and high spin complexes - Pairing energy - Spin cross-over region - Brief account of transition elements

**ORGANOMETALLIC CHEMISTRY:** **[3 h]**

Definition, nomenclature and classification of organometallic compounds- Alkyl and aryls of Li, Al, Hg and Sn- Metal-ethylenic complexes

**BIOINORGANIC CHEMISTRY:** **[3 h]**

Essential and trace elements in biological processes- Oxygen transport in myoglobin and haemoglobin- Biological function of alkali metal ions

**Suggested Text Books**:

F. A. Cotton, G. Wilkinson, P. G. Gauss, Basic Inorganic Chemistry, 3rd Edition, John Wiley, 1995

**Course Code : CY302**
**Title of the Course : Organic Chemistry: Synthesis and Reactions**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** A course on Basic Organic Chemistry

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the behavior of various functional groups in organic chemistry

**CLO-2 :** explain how chemical reactions proceed under different conditions

**CLO-3 :** apply in deriving mechanism of chemical transformations

**CLO-4 :** apply the known reactions to deduce synthetic methods for the target molecules

**CLO-5 :** propose possible mechanism for novel transformations

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 2 | 1 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 1 | 2 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 2 | 1 | 2 | 2 |

## Detailed Syllabus (CY302)

Addition to C=C bonds and organometallics (8 h)

Electrophilic addition to C=C bonds: Mechanism, reactivity, regioselectivity and stereoselectivity. Reactions: halogenation, hydrohalogenation, hydration, hydrogenation, epoxidation, hydroxylation, ozonolysis, electrophilic addition to dienes (conjugated dienes and allenes). Cycloaddition.

Radical addition: HBr addition, dissolving metal reaction of alkynes and benzenoid aromatics (Birch).

Organometallics: preparation of Grignard reagent, organo lithium and Gilman cuprates and their reactions, 1,2- and 1,4-additions. Reformatsky reaction.

Chemistry of carbonyl compounds (9 h)

Chemistry of -carbon of carbonyls--hydrogen (pKa of different carbon acids), keto-enol tautomerism, base and acid catalyzed keto-enol tautomerism. Halogenation, haloform reaction, Hell-Volhardt--alkylation, aldol reaction [mixed and directed (metal enolate, enamine)], Michael reaction, Robinson annulation, Knoevenagel condensation, Claisen ester condensation, Dieckmann condensation, Perkin reaction, Stobbe condensation, Darzens reaction, acyloin condensation, McMurry coupling, Wittig reaction.

Malonic and acetoacetic esters: Characteristic reactions of active methylene group, synthetic uses of malonic, acetoacetic and cyanoacetic ester.

Addition of nucleophile to carbonyl adjacent to stereogenic center: Cram and Felkin-Anh model. Umpolung using dithiane.

Reagents for reduction and oxidation: Classical methods. (6 h)

Substitution, and elimination reactions (13 h)

Substitution at sp3 carbon center- $S_N1$, $S_N2$ and $S_N2'$ mechanisms), effect of solvent, substrate structure, leaving group and nucleophiles, including ambident nucleophiles (e.g. cyanide & nitrite). Mechanism: E1, E2 and E1cB; reactivity. Substitution involving NGP, relative rate & stereochemical features [systems: alkyl halides, allyl halides, alcohols, ethers, epoxides]. Substitution at sp2 carbon. BAC2, AAC2, AAC1 and AAL1 mechanisms (in connection with acids and esters), nucleophilic substitution (SN1, SN2 NGP) cyclohexane system. Elimination (E2) in cyclohexane system. Stereoselective approach to E1, E2 and E1cB mechanisms; reactivity/ orientation (Saytzeff/Hofmann).

Electrophilic aromatic substitution: mechanism orientation and reactivity. Reaction: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction, chloromethylation, Gatterman, Hoesch, Vilsmeier-Haack reaction, Reimer-Tiemann, Kolbe-Schmidt. Nucleophilic substitution reaction: Addition-elimination reaction. SN1 mechanism, benzyne mechanism.

**Suggested Text Books:**

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
4. I. L. Finar, Organic Chemistry, Vol-1, 6th edition, Pearson Education.
5. S. N. Ege, Organic Chemistry: Structure and Reactivity, 5th edition, Houghton Mifflin College Div, 2003.
6. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley.

**Course Code : CY303**
**Title of the Course : Analytical Chemistry**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY101

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of errors in chemical analysis, more specifically, how to report the analyzed data.

**CLO-2 :** understand the basic principles of acid-base titrations, redox titrations, precipitation titrations, complexometric titrations and electrochemical analyses.

**CLO-3 :** understand the basic principles of solvent extractions and diverse chromatographic techniques.

**CLO-4 :** solve stoichiometric calculations / mathematical problems, related to acid-base titrations, redox titrations, precipitation titrations, complexometric titrations and electrochemical analyses.

**CLO-5 :** apply this overall knowledge of analytical chemistry to handle industrial, pharmaceutical and biochemistry problems including problems in daily life chemistry.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 1 | 3 | 2 | 3 | 3 | 2 |
| **CLO-2** | 3 | 2 | 1 | 3 | 3 | 3 | 2 | 3 |
| **CLO-3** | 2 | 2 | 2 | 3 | 2 | 3 | 2 | 3 |
| **CLO-4** | 2 | 2 | 3 | 3 | 2 | 2 | 3 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 2 | 3 | 3 | 3 |

## Detailed Syllabus (CY303)

Errors in Chemical Analysis (6 h)

Errors and types - Accuracy and precision, Absolute and relative errors, Determinate (systematic) and indeterminate (random) errors,

Statistical treatment of random errors – source and distribution, sample and populations, mean, deviations and standard deviation. Propagation of errors, criteria for rejection of a data (q-test), significant figure and computation rules for significant figures, method of least squares.

Acid-base Titrations (6 h)

Terminology– equivalence point and end point, primary and secondary standards, reactions used for titrations, molarity and normality, some examples of stoichiometric calculations.

Acid-base titration– Acid-bas indicators, theory of acid base indicators, calculation of pH values at different stages of the acid base titration and titration curve.

Precipitation and Complexometric Titration (6 h)

Precipitation titrations- mohr, volhard and fajans methods with examples and indicator theory.

Complexometric titrations- principle, effect of complexing agents and their advantages, examples including EDTA based titration and titration curve, definition of pM+ (-log M+), Back and blank titration with examples, direct and indirect determinations, masking and demasking with examples

Gravimetric Method of Analysis (4 h)

Gravimetry– principle and use with example, Von weimern theory of relative supersaturation, digestion-ostwald ripening, coprecipitation, post precipitation, precipitation from homogeneous solution, organic precipitants.

Electrochemistry in Analysis (8 h)

Redox titrations – Redox indicators, their use in volumetric analysis, iodometry and iodimetry, example of titration from other redox systems.

Electrochemical methods – electrodes and electrochemical cell, standard electrodes, electrochemical series, glass electrode and pH measurement, electrogravimetry, potentiometric titration, DME and polarography, cyclic voltammetry.

Separation Techniques (8 h)

Solvent extraction, gas-liquid chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography.

**Suggested reading:**

(1) "Qualitative Analysis" – Day and Underwood, 5th edition, Prentice-Hall (1986).

(2) "Fundamentals of Analytical Chemistry" – Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, 9th Edition,Cengage Learning(2013

**Course Code : CY304**
**Title of the Course : Surface Chemistry and Electrochemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** IMSc courses in the I - IV semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the surface, interface, basic conduction phenomenon

**CLO-2 :** provide insight into the various classes of reactive surface, isotherms, electrical conduction behavior.

**CLO-3 :** understand and analyze migrations of ions, isotherms, electrode potentials

**CLO-4 :** apply the basic concept of surface, interface and electrochemistry for various physical insights.

**CLO-5 :** apply the electrochemistry concept in designing new cells.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 2 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 2 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY304)

Surfaces and interfaces: surface free energy and surface tension, contact angles and wetting, work of adhesion and cohesion, curved interface, Young's equation, capillary action, surfactants and surface pressure, surface excess, Gibbs isotherm, surface double layer and potential. **(6 h)**

Structure of solid surfaces: Adsorption and desorption of molecules, physisorption and chemisorption, Langmuir Isotherm, BET and other isotherms, dissociative adsorption, temperature dependence of adsorption, sticking probability. Surface analytical techniques, spectroscopies (Auger, photoelectron, vibrational) temperature programmed techniques. Surface imaging electron microscopy. **(6 h)**

Reactions at surfaces: heterogeneous catalysis, Langmuir-Hinshelwood and Eley-Rideal mechanisms, activation energy. **(3 h)**

Relevance of surfaces and interfaces: colloids, nanomaterials & biology. **(2 h)**

Conductance and Ionisation: ionic conductance, electrical force, field and flux, molar conductivity, strong and weak electrolytes and their molar conductance, law of independent migration of ions: Kohlrausch's law, Ostwald's dilution law, conductometric titrations. **(4 h)**

Theory of Electrolytic Conductance (qualitative description only): ionic atmosphere, electrophoretic effect - Debye-Hückel-Onsager equation, Effect of high potential gradient (Wien effect) and high frequency (Debye-Falkenhagen effect). **(4 h)**

Migration of Ions: Ionic mobility, drift speed, Transport number and its relation with concentration and ionic mobility, Experimental procedures for measuring transport numbers (Hittorf's rule, Moving boundary method), Abnormal transport numbers: Grotthuss mechanism. **(3 h)**

Ion Activities and Debye-Hückel Theory (qualitative descriptions only): Activity and activity coefficients, Ionic strength, Debye-Hückel limiting law, Debye-Hückel theory for concentrated solution. **(3 h)**

Electrochemical Cells: Daniell Reversible and irreversible cells, cell representations and half-cell reactions, E.M.F., Thermodynamics of electrochemical systems: Nernst equations, varieties of electrodes, standard electrode potential. **(3 h)**

Type of boundary between half cells and Liquid junction potentials, Concentration cells, Applications of EMF measurements- potentiometric titrations, determination of activity coefficient, composition of complex ions, solubility product, measurement of pH and pKa (Hydrogen, Quinhydrone, Glass electrodes), Polarization, Overvoltage **(3 h)**

Application of Electrochemical Cells- Dry cells, Lead Batteries, Alkaline cells (Edison Cell), Fuel cells, Biological energy conversions. **(3 h)**

**Suggested readings:**

1. Physical Chemistry- P. W. Atkins
2. Electrochemistry – Samuel Glasstone

**Course Code : CY305**
**Title of the Course : Organic Chemistry: Conformation and Reactivity**

**L-T-P** : L ~~/ T / P~~

**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** A course on basic understanding of reaction kinetics, conformation and heterocycles (Physical Aspects)

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of reaction kinetics and thermodynamics.

**CLO-2 :** understand conformation of a molecule and how they affect the reactivity.

**CLO-3 :** understand the basic principles of photochemistry.

**CLO-4 :** know the photochemical reactions.

**CLO-5 :** understand the impact of aromatic and heteroaromatic compounds in synthesis.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-2** | 3 | 2 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 2 | 2 | 1 | 3 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 3 | 3 | 3 | 3 |

## Detailed syllabus (CY305)

**Thermodynamic and kinetic principles** [11 h]

Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factors, intermolecular and intramolecular reaction. Heat of hydrogenation and heat of combustion. Application of thermodynamic principle in tautomeric equilibria [keto-enol tautomerism, composition of the equilibrium in different systems (simple carbonyls, 1,3- and 1,2-dicarbonyl systems, phenols, and related systems), substituent and solvent effects]. Reaction kinetics; transition state theory, rate constant and free energy of activation, free energy profile for one step and two step reactions, catalytic reactions, kinetically controlled and thermodynamically controlled reactions, isotope effect, primary kinetic isotopic effect (kH/kD), principle of microscopic reversibility. Crossover experiments.

**Conformation and stereochemistry** [13 h]

Racemization (through cationic, anionic and radical intermediates), resolution of acids, bases and alcohols via diastereomeric salt formation. Topicity of ligands and faces; Pro-R, Pro-S, and Re/Si descriptors.

Conformation : nomenclature, eclipsed, staggered, gauche and anti, dihedral angle, torsion angle, energy barrier of rotation, relative stability of conformation on the basis of steric effect, dipole-dipole interaction, H-bonding; conformational analysis of ethane, propane, n-butane, haloethane, 1,2-haloethane, 1,2-glycol, 1,2-halohydrin; invertomerism of trialkylamine.

Cyclic stereochemistry: Baeyer strain theory, conformational analysis: cyclohexane, mono and disubstituted cyclohexane, symmetry properties, and optical activity.

**Photochemistry** [4 h]

Primary photochemical processes, Jablonskii diagram, photochemical reactions of carbonyl compounds: Norrish type I and II reactions. Photochemistry of olefins: cis-trans isomerism, Paterno-Buchi reaction.

**Aromatic and Heterocyclic compounds** [8 h]

Naphthalene, anthracene and phenanthrene. Heterocyclic compounds: synthesis, structure, reactivity, orientation and important reactions of epoxide, aziridine, furan, pyrrole, thiophene, and pyridine.

**Suggested Text Books:**

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. M. B. Smith and J. March, March's Advanced Organic Chemistry, 6th edition, Wiley, 2007.
4. 5. Jonathan Clayden, Nick Greeves, Stuart Warren: Organic Chemistry 2nd Edition, Oxford, 2014

**Course Code : CY306**
**Title of the Course : Organic Chemistry Lab**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 2

**Prerequisite Course / Knowledge (If any):** CY252

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** provide insight into organic chemistry lab

**CLO-2 :** appreciate the basic concepts related to the synthesis of organic compounds

**CLO-3 :** apply the basic concepts of new organic compounds based on a fundamental understanding

**CLO-4 :** practice laboratory safety

**CLO-5 :** apply different synthetic techniques for the synthesis of organic compounds

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY-306)

Preparation of organic compounds using classical organic reactions such as nitration, bromination, acetylation, condensation and oxidation.
Estimation of selected organic compounds.

**Suggested reading:**

1. A.I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.
2. Laboratory manual.

**Course Code : CY307**
**Title of the Course : Analytical Chemistry Lab**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 2

**Prerequisite Course / Knowledge (If any):** Basic analytical chemistry course

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the concentrations, molarity, volumetric and gravimetric methods.

**CLO-2 :** explain how volumetric and gravimetric analysis are useful to find out a amount of particular cations/anions in Food and other materials.

**CLO-3 :** apply the various analytical approaches for quantitative measurements.

**CLO-4 :** apply quantitative concepts to analyze the unknown amount in the samples including drugs to cooking materials.

**CLO-5 :** create a new quantitative approach from learned analytical approach.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY307)

Food, Fertilizer and cosmetics analysis

1. Determination of the amount of calcium in milk powder by EDTA complexometric titration.

2. Estimation of iodine in iodized common salt using iodometric titration.

3. Estimation of phosphoric acid in cola drinks (coke, thumps up and Pepsi) by blue phosphomolybdic acid method (spectrophotometry).

4. Analysis of phosphorous (as phosphate) from phosphorous containing fertilizer.

5. Analysis of sulfur (as sulfate) from sulfur containing fertilizer.

6. Gravimetric analysis of aluminum in commercially available deodorants.

7. Preparation of [Ni(NH3)6]2+ and analysis of its nickel content by gravimetric method.

8. Extraction and identification of DNA from green peas.

9. Analysis of kidney stones by permanganometric titration.

10. Determination of hardness of tap water.

**Reference Books:**


5) Anil J. Elias (2002), A collection of interesting GENRAL CHEMISTRY EXPERIMENTS, Universities Press.
6) (1989), Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn, Orient Longman.
7) Laboratory Manual
8) Papers from Chemical Education Journals.

**Course Code : CY351**
**Title of the Course : Instrumental Methods of Analysis**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** None

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** observe and recognize the basics of different instruments design and function (various Mass spectrometry, X-Ray diffraction techniques, UV-IR-Raman-CD, NMR, EPR, atomic absorption/emission spectroscopy) for chemical analysis.

**CLO-2 :** understand and recognize various electronic/optical/magnetic/electric components of various instruments from a chemical perspective.

**CLO-3 :** realize the concepts of various instrumental techniques for the analysis of diverse chemical compounds in various forms (crystals/films/powder).

**CLO-4 :** design a combination of different instrumental techniques to analyses the chemicals.

**CLO-5 :** understand the importance of design and development of new instrumental techniques for societal needs.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 2 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 2 | 2 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 2 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 1 | 3 | 3 |
| **CLO-5** | 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY351)

Introductory treatment of the following techniques, including basic instrumentation and illustrative applications from all branches of chemistry.

Absorption and emission spectroscopy (8 h)

Atomic spectroscopy – instrumentation of AAS, AES, ICP-MS/AES Molecular spectroscopy – instrumentation of UV-Vis, IR and CD spectroscopy

Mass spectrometry (8 h)

Basic treatment of ionization methods – FD, EI, CI, ESI, MALDI, FAB Mass analyzers – sectors, quadruple, TOF, ion trap, Detectors – electron multiplier, Faraday cup, array detectors Applications – small molecules, inorganic complexes, polymers, proteins

NMR spectroscopy (8 h)

Basics – Larmor precession, resonance absorption, magnetic fields, shielding and chemical shifts, chemical equivalence, relaxation processes Solution state ($^{1}H$, $^{13}C$) and solid state techniques Instrumentation – block diagram, magnets, sample probe, RF generation and detection,

FT NMR/ESR spectroscopy (6 h)

Introduction – g factor, hyperfine coupling, fine structure Instrumentation – microwaves, waveguides, magnetic field modulation Applications – free radicals, metal complexes, reaction intermediates

Diffraction Techniques (8 h)

X-ray diffraction – Crystal lattices and Miller planes, Bragg condition, Ewald's sphere Instrumentation – X-ray sources including synchrotron, filters, detectors including CCD ,Powder diffraction techniques – Debye-Scherrer Single crystal data collection – 4-circle method, Laue method, rotating crystal

**Suggested Reading:**


1. Undergraduate Instrumental Analysis by James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, Sixth Ed, Marcel Dekker, New York, 2005.
2. . Introduction to Spectroscopy by Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, Fourth Ed., Brooks/Cole Thomson Learning 2009.
3. 3. Physical Chemistry by Peter Atkins and Julio de Paula, 9th Ed., Oxford University Press, 2010.
4. 4. Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds by William Henderson and J. Scott McIndoe, John Wiley & Sons Ltd, 2005.

**Course Code : CY352**
**Title of the Course : Industrial and Environmental Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** basic chemistry knowledge

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** provide insight into fuel classification

**CLO-2 :** provide insight into petrochemical and catalysis

**CLO-3 :** appreciate the industrial organic synthetic processes

**CLO-4 :** appreciate the chemistry behind essential commodities such as soap, polymer, cement etc..

**CLO-5 :** provide insight into Green Chemistry and synthesis

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 1 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 1 | 3 |

## Detailed Syllabus (CY352)

Fuels: Classification, solid, liquid, and gaseous forms. Occurrence, purification, composition and calorific value **[2 h]**

Petrochemicals and petroleum products **[4 h]**

Catalysis: Relevant to industrial applications. **[2 h]**

Industrial organic synthesis: Synthesis of methanol, ethanol, acetic acid, acetone, glycerol and ethyl acetate etc **[3 h]**

Silicates, glass, ceramics, refractories, cement. **[3 h]**

Fertilizers: Nitrogenous and phosphate fertilizers. **[3 h]**

Industrial acids and bases **[2 h]**

Active pharmaceutical intermediates and drugs **[2 h]**

Polymers, plastics, rubber, synthetic fibers, and paper [**4 h**]

Soaps and detergents [**2 h**]

Insecticides and pesticides [**2 h**]

Dyes, paints and pigments [**2 h**]

Tanning of leather [**2 h**]

Environmental aspects: Global warming, acid rains, smog, ozone depletion, toxic metals, carcinogens. Green chemistry [**3 h]**

**Suggested Reading:**


1. P. J. Chenier, Survey of industrial chemistry, 3rd Edition, Kluwer Academic/Plenum Publishers, 2002.
2. B. K. Sharma, Industrial Chemistry including Chemical Engineering, Krishna Prakashan Media (p) Ltd, 2006.
3. S. E. Manahan, Fundamentals of Environmental Chemistry, 3rd edition, CRC press, 2008.


***Web resource:*** http://chemistry.uohyd.ac.in/~CY352/

**Course Code : CY354**
**Title of the Course : Computer Programming and Numerical Methods**

**L-T-P** : L / T / P
**Credits** : 2 – 0 – 1

**Prerequisite Course / Knowledge (If any):** basic graduation level knowledge of chemistry and mathematics mandatory. Knowledge of programming language is plus point, but not mandatory.

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of different numerical methods and equip them to apply numerical methods to obtain approximate solutions to mathematical problems.

**CLO-2 :** write simple, error free computer programs and equip them to develop simple numerical algorithms.

**CLO-3 :** learn the basics of Fortran programing language and acquire the skill to implement numerical methods in Fortran language.

**CLO-4 :** learn the basics of python programming language and acquire the skill to implement numerical methods in python language.

**CLO-5 :** apply the acquired skills to design new algorithms and write efficient computer programs and master the art of scientific programming.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 3 | 3 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY354)

Computer: brief description of Hardware & Software. Programming in FORTRAN: Program design (algorithm), organization of program, data types and integer constants, complex constants, logical constants, variables, implicit and explicit data typing, expressions and hierarchy of operations, mix-mode arithmetic, library functions, input/output specification, formatting, unconditional transfers, conditional statements and constructs, GO TO/ IF statements, relational operators, block if structure, else if construct, do loops, nesting, variables and arrays, parameter/data statements, common blocks, read/write by opening files, subroutines and construction of large program.

Programming Laboratory (Linux OS, vi editor): Students are instructed to write programs of the numerical methods taught.

Numerical Methods: Taylor's theorem, Expansion of functions, Remainder, Mean value and Extreme value theorems, Discrete average value theorem. Numerical Differentiation (first, second and higher derivatives)- Truncation and Round-off errors, Step-size dilema, Difference table (Pascal's triangle). Numerical Integration- Riemann sum, Quadrature rule, Interpolating polynomials (Lagrange's), Weights, Mid-point, Trapezoidal, Simpson's rule of integration, Adams' Predictor-Corrector method. Roots of equations- Newton-Raphson and Secant methods, Bisection and False-point methods, Bracketing method. Numerical solution of ordinary differential equations- Initial value problems, Euler's method, Taylor and Runge-Kutta methods, Modified Euler and Huen's method, Error estimates. Curve fitting- Least square fit algorithm, Monotone and convex data. Linear systems- Forward, Backward substitution, LU- factorization, pivoting (only basics), Gaussian Elimination, Gauss-Jordan Elimination, Jacobi and Gauss-Seidel methods. Eigenvalue problems. Statistical analysis of data.

**Suggested reading:**

1. Numerical Analysis: a Mathematical Introduction, M. Schatzman, Oxford University Press.
2. Numerical Methods in Fortran, J. M. McCormick and M. G. Salvadori, Prentice Hall of India Private Limited.
3. Numerical Analysis, R. L. Burden and J. D. Faires, Brooks/Cole Thomson Learning. 4. An Introduction to Numerical Methods and Analysis, J. F. Epperson, John Wiley and Sons, Inc.
5. Numerical Analysis: A Practical Approach, M. J. Maron, Macmillan Publishing Co. Inc.
6. Introduction to Numerical Analysis, F. B. Hildebrand, McGraw Hill Book Company, New York.
7. Numerical Methods for Engineers, D. V. Griffiths and I. M. Smith, Oxford University Press.
8. Fortran 77 and Numerical Methods, C. Xavier, New Age International Publishers.
9. Computer Programming in Fortran, V. Rajaraman, PHI Learning Private Limited.
10. Numerical Analysis and Computational Programming, S. A. Mollah, Books and Allied (P) Ltd.
11. Numerical Recipes in Fortran: The art of Scientific Computing, W. H. Press, S. A. Teukolsky, W. T. Vellerling and B. P. Flannery, Cambridge University Press.

**Course Code : CY355**
**Title of the Course : Inorganic Chemistry Laboratory (2 credits)**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 2

**Prerequisite Course / Knowledge (If any):** NIL

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** synthesize Werner-type coordination compounds

**CLO-2 :** analyze and understand the structure of the synthesized compounds

**CLO-3 :** develop skills of growing single crystals suitable for diffraction technique

**CLO-4 :** design and synthesize main group metal based compounds

**CLO-5 :** utilize the skills acquired for designing and synthesizing novel molecular frameworks.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY355)

Synthesis of a variety of Inorganic Compounds:

Complexes of 3d metal ions and rare earth ions and main group compounds by using common experimental techniques.

Study of the related literature (UG level).

Preparation of Scientific Reports.

**Course Code : CY356**
**Title of the Course : Industrial Chemistry Laboratory**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 2

**Prerequisite Course / Knowledge (If any):** IMSc courses in the I – V semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** provide insight into industrial chemistry

**CLO-2 :** appreciate the basic concepts related to the industrial chemistry

**CLO-3 :** apply the basic concepts of new industrial chemicals based on a fundamental understanding

**CLO-4 :** understand the synthesis of industrial compounds

**CLO-5 :** apply different synthetic techniques for synthesis of industrial compounds

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY356)

Experiments based on major industrial processes, operations and methods of analysis of Industrial Chemicals and materials.

1. Synthesis of allobarbital
2. Synthesis of warfarin
3. Synthesis of paracetamol
4. Synthesis of oil of wintergreen
5. Synthesis of indigo and dyeing of cloth
6. Extraction of casein from milk
7. Estimation of iron in tablet
8. Extraction of curcumin from turmeric
9. Preparation of soap
10. Laboratory preparation of shaving gel
11. Preparation of nylon 6 6
12. Preparation of super absorbent polymer and exploration of its properties
13. Synthesis of molecular sieve – zeolite X and cobalt exchange reaction with it
14. Synthesis of biodiesel

**Course Code : CY357**
**Title of the Course : Open-ended Laboratory**

**L-T-P** : ~~L / T~~ / P

**Credits** : 0 – 0 – 2

**Prerequisite Course / Knowledge (If any):** Basic chemistry knowledge

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** learn how to approach a research problem

**CLO-2 :** direct the student to independent thinking

**CLO-3 :** learn frontier areas of chemical research

**CLO-4 :** apply the ideas to design new experiments

**CLO-5 :** learn to handle few sophisticated equipment

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 1 | 3 | 3 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 1 | 3 | 3 |

## Detailed syllabus (CY357)

In this course, students are assigned a task and are expected to try various approaches to solve it. For example, enzyme kinetics studies, study of the gel-fluid phase transition of lipids using fluorescence, organic synthesis and synthesis of giant inorganic metal oxide clusters and their reactions. The students are assessed based on the practical skills in the lab, originality and the written report at the end of the course. Since the course in the nature of short projects, the experiments chosen may vary from year to year.

**Reference Books:**

Lab manual, provided by the course instructor

**Course Code : CY401**
**Title of the Course : Basic Concepts and Coordination Chemistry (3 credits)**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** NIL

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of inorganic and coordination chemistry

**CLO-2 :** understand and analyse inorganic reaction pathways using redox data

**CLO-3 :** understand and analyse structure-property correlation of coordination compounds

**CLO-4 :** design new coordination compounds based on a fundamental understanding of their electronic properties

**CLO-5 :** appreciate specialized and advanced topics in inorganic and coordination chemistry.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 1 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 2 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY401)

**Shapes of Small Molecules:** VSEPR theory - Coordination polyhedra - Enumeration of geometrical and optical isomers. (3 h)

**Theory of Acids and Bases:** Bronsted and Lewis acids and bases - Gas phase versus solution acidity - Solvent leveling effects - Hardness and softness - Surface acidity. (5 h)

**Oxidation and Reduction:** Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials - Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams. (6 h)

**Coordination Chemistry:** d-orbital splitting in various fields – Spectroscopic states and term symbols - Hole formalism - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq. B) from electronic spectra - Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries - Bonding involving pi-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements. (18 h)

**Inorganic Reaction Mechanisms:** Substitution reactions - Dissociative and associative interchange - trans -effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and -redox reactions, Fluxional molecules. (8 h)

**Suggested reading:**

(1) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Edn, OUP, 1999.
(2) C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(3) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Edn Wiley, 1999).
(4) J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Edn, Prentice Hall, 1997 (or a previous edition).
(5) G. L. Miessler, D. A. Tarr, ''Inorganic Chemistry'', 3rd Edn, Pearson Education, 2004.
(6) G. Wulfsberg, ''Inorganic Chemistry'', University Science Books, 2000.

**Course Code : CY402**
**Title of the Course : Physical Organic Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** BSc Organic Chemistry

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** Provide insight into physical concepts of structure and bonding

**CLO-2 :** Appreciate the basic concepts related to the structure and reactivity

**CLO-3 :** Provide insight into aromaticity

**CLO-4 :** Discussion and predicting the reactivity based on physical concepts

**CLO-5 :** Detailed discussion and understanding of stereochemistry and synthesis

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 2 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY402)

Structure and bonding: Description of molecular structure using valence bond concept (Hybridization, bond lengths and angles). **[2 h]**

M.O. and V.B. methods (Huckel's MO Method, pictorial representation of MOs for molecules, Qualitative application of MO theory to reactivity). **[5 h]**

Inductive, resonance, hyperconjugation and field effects, hydrogen bonding. **[2 h]**

Aromaticity and Huckel's rule (energy, structural, electronic criteria for aromaticity and relationship among them, aromaticity for annulenes, charged rings, homoaromaticity, fused rings, heteroaromaticiy). **[4 h]**

Thermodynamics and kinetics: Acids and bases, HSAB principle, bond energies and thermochemistry, kinetic parameters, Hammond's postulate, Kinetic isotope effects, kinetic and thermodynamic control (general relationship between thermodynamic stability and reaction rate). **[7 h]**

Linear free energy relationships for substituent effects (numerical expression and application to characterization of reaction mechanisms). **[4 h]**

Stereochemistry: Chirality and isomerism in organic systems, resolution and asymmetric synthesis, conformational analysis of acyclic and cyclic systems, Curtin-Hammett principle. Effect of Conformation on reactivity: stereo electronic effects. **[10 h]**

Supramolecular chemistry: Host-guest systems, crowns, cryptands, clathrates and inclusion complexes. **[2 h]**

**Suggested Reading:**


1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
2. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry Illustrated Edition, University Science, 2005.
3. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
4. A. J. Kirby, Stereoelectronic Effects, Oxford University Press, 1996.
5. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
6. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds Wiley Student Edition, 2008.


***Web resource:*** http://chemistry.uohyd.ac.in/~CY402/

**Course Code : CY403**
**Title of the Course : Quantum Chemistry**

**L-T-P :**L / T / P
**Credits :** 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** Basic mathematics, differential equations, orthogonal polynomials, matrix algebra, group theory and character tables

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1:** This is a course that introduces students to understand chemistry at a molecular level applicable to all branches of chemistry and physics.

**CLO-2 :** New mathematical techniques are introduced. Success and shortcomings of the theory is discussed. The students would learn to interpret modern experiments in spectroscopy and chemical dynamics.

**CLO-3:** Basic foundation of quantum mechanics is introduced. Tool to arrive at practical computations is covered. This helps students to carry out hands-on experiments in computational chemistry.

**CLO-4 :** Symmetry plays a major role in science and technology. Students would appreciate to simplify complex problems with the aid of symmetry. The idea of quantum tunneling of practical relevance and spin of microscopic particles would provide further insights into this new mechanics.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs) and Program Specific Outcomes (PSOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 3 | 3 | 1 | 2 | 2 | 2 |
| **CLO-2** | 3 | 1 | 2 | 3 | 1 | 2 | 2 | 2 |
| **CLO-3** | 3 | 1 | 1 | 3 | 1 | 2 | 3 | 3 |
| **CLO-4** | 3 | 1 | 1 | 3 | 1 | 2 | 3 | 3 |

## Detailed Syllabus (CY403)

Review of classical mechanics. Wave-particle duality and Uncertainty principle.

Postulates of quantum mechanics. Operator algebra. Properties of hermitian operators. Eigenvalue problem. Commutators and Uncertainty Principle.
Elementary applications of quantum mechanics- unbound motion in one dimension. Tunneling. Bound motion – particle-in-a-box (1D & 3D), harmonic oscillator and rigid rotor. Angular momentum algebra- Hydrogen atom.
Methods of obtaining approximate solution to the time independent Schrödinger equation – perturbation theory and variational method. Application.
Many electron atoms. Spin and Pauli exclusion principle. Hund's rule. Slater determinants. Electronic term symbols.

Suggested reading:

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
2. Quantum Chemistry, D. A. McQuarrie, University Science Books.
3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Quantum Mechanics, L. Pauling and E. B. Wilson,McGraw Hill International Ed.
5. Quantum Mechanics, N. Zettili, John Wiley and Sons.
6. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
7. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
8. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

**Course Code : CY404**
**Title of the Course : Symmetry, Group Theory and Mathematics**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** basic graduation level knowledge of mathematics expected but not mandatory.

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand basic and different areas of mathematics.

**CLO-2 :** nurture a mathematical aptitude, thinking, and inculcate skills to solve problems.

**CLO-3 :** inculcate mathematical reasoning and enable them to understand the mathematical models in chemistry.

**CLO-4 :** prepare the students to apply the mathematics knowledge in learning and understanding other courses in physical and inorganic chemistry better, especially like quantum chemistry and molecular spectroscopy etc.

**CLO-5 :** learn the basics of group theory and its application in chemistry. This knowledge may equip them to learn other courses in M.Sc. Chemistry like spectroscopy and coordination chemistry etc.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 3 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 3 | 1 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 3 | 3 | 1 | 3 |

## Detailed Syllabus (CY404)

Prerequisite: Basic Mathematics

Symmetry elements and operations; matrix representation of symmetry operations; properties of groups and point groups; reducible and irreducible representations, Great Orthogonality Theorem, construction of character tables; direct product representations; projection operators and symmetry adapted linear combinations. Applications to mean observables in molecular spectroscopy. Introduction to molecular space group.

Real and Complex number algebra, Vector algebra: products of vectors, orthonormal vectors; Sequences and series: finite & infinite series, MacLaurin & Taylor series.

Determinants and Matrices: properties of determinants, matrix algebra, orthogonal transformation, rank and inverse of matrix, eigenvalues and eigenvectors.

Functions and variables': limits and continuity; Differential calculus: first- & higher-order derivatives, minima and maxima, partial differentiations, exact and inexact differentials.

Integral Calculus: Indefinite and definite integrals, improper integrals, methods of integration.

Differential Equations: ordinary first- and second-order differential equations and their method of solutions, power series method, Hermite, Legendre, Laguerre and Bessel equations, partial differential equations, Fourier series and transforms.

Probability and Statistics: permutation & combination, discrete and continuous probability distribution functions, joint and conditional probability distributions, moment and error calculations.

**Suggested Reading:**


1. Symmetry and Group Theory in Chemistry, Mark Ladd, Horwood Publishing Limited
2. Molecular Symmetry and Group Theory. Allan Vincent, John Wiley & Sons, LTD.
3. Symmetry: An introduction to group theory and its applications. R. McWeeny, Dover Publications, Inc.
4. Chemical Applications of Group Theory. F. A. Cotton, John Wiley & Sons, Inc.
5. Symmetry and Structure. S. F. A. Kettle, Wiley.
6. Group Theory in Chemistry: Bonding and Molecular Spectroscopy by Ghosh and Mukherjee
7. Advanced Engineering Mathematics. E. Kreyszig, Wiley.
8. The Chemistry Maths Book, E. Steiner, 2nd Ed., Oxford University Press
9. Mathematics for Physical Chemistry. R. G. Mortimer, Academic Press.
10. Mathematics for Chemistry and Physics. G. Turrell, Academic Press.
11. G. Stephenson, Mathematical Methods for Science Students (510.245 St44M)
12. H. H. Jaffè and M. Orchin, Symmetry in Chemistry (541.2 J18S)

**Course Code : CY405**
**Title of the Course : Inorganic Chemistry Lab: Quantitative and Qualitative Analysis**

**L-T-P** : ~~L / T~~/-P
**Credits** : 0– 0 –3

**Prerequisite Course / Knowledge (If any):** Basics of Chemistry (undergraduate)

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1:** analyze common chemicals for their identity and composition

**CLO-2:** appreciate the strengths and limitations of various physical techniques to analyze chemicals

**CLO-3:** have hands-on experience/practical knowledge in performing experiments

**CLO-4:** separate different metal ions on the basis of their reactivity by checking the reactivity

**CLO-5:** design/modify the existing set up for chemical analysis

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 2 | 1 | 3 | 2 | 2 | 2 |
| **CLO-2** | 2 | 2 | 2 | 1 | 2 | 1 | 2 | 2 |
| **CLO-3** | 3 | 2 | 2 | 2 | 1 | 2 | 2 | 3 |
| **CLO-4** | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 3 |
| **CLO-5** | 2 | 3 | 3 | 2 | 2 | 2 | 2 | 3 |

## Detailed Syllabus (CY405)

Quantitative Analysis
Statistical analysis of data sampling methods.
Redox titrations (permanganometry, dichromatometry, iodometry).
Complexometric titrations using EDTA (estimation of some metal ions, hardness of water).
Precipitation titration (estimation of Ag).
Quantitative separation of metal ions from a binary mixture (e.g. Cu2+/Fe3+).
Gravimetric analysis (e.g. estimation of Ni2+).
Analysis of ores and minerals (e. g. Iron ore, Potassium alum).
Ion exchange separation of metal ions (e.g. Zn2+/Mg2+).
Ion exchange separation of oxidation states (e.g. VO3 /VO2+).
Qualitative Analysis
Reactions of some less common metal ions (TI, W, Mo, V, Zr, Th, U).
Simple reactions to illustrate the aqueous chemistry of some typical transition metal ions - several oxidation states of V, Cr, Mn - oxoions - Peroxo ions; complex formation of Co2+ - H2O-HCl reaction.
Group separation of cations (mostly trace elements).

**Suggested reading:**

(1) Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn, Orient Longman, 1989.
(2) Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, 5th Edn, Orient Longman, 1982.

**Course Code : CY406**
**Title of the Course : Advanced Organic Chemistry Lab**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 3

**Prerequisite Course / Knowledge (If any):** None

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to …**

**CLO-1 :** determine the melting point of pure organic solids

**CLO-2 :** purify impure organic solids by recrystallization or sublimation

**CLO-3 :** purify/separate organic liquids by simple and fractional distillation

**CLO-4 :** verify the purity of organic compounds/identify the number of organic compounds in a mixture employing thin layer chromatography

**CLO-5 :** purify/separate organic compounds by column chromatography

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 3 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |

## Detailed Syllabus (CY406)

Prerequisite:

Different laboratory techniques: TLC, column chromatography, separation and analysis of organic compounds.

Multistep organic synthesis involving oxidation, reduction, electrophilic substitution, organometallic reagents, cycloaddition, photochemical, rearrangements, radical and enzymatic reactions.

Resolution of racemic organic compounds.

Characterization of the synthesized compounds using different analytical techniques.

Suggested reading:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz and R. G. Engel, A Microscale Approach to Organic Laboratory Techniques, 6 th Edition, Cengage Learning, ELBS (2016).

2. A. I. Vogel, Textbook of Practical Organic Chemistry, 4 th edition.

3. Laboratory manual.

**Course Code : CY451**
**Title of the Course : Main Group and Inner Transition Elements**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc course CY401

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1:** analyze the position, periodicity and properties of main group elements and inner transition elements.

**CLO-2:** comprehend why elements behave the way they do and analyzing the apparent anomalies

**CLO-3:** get information on new reactions and pathways for future uses, if any

**CLO-4:** search the literature through textbooks or e-resources on the subject

**CLO-5:** appreciate advanced topics in the subject for future applications

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 2 | 1 | 3 | 3 | 1 | 1 | 1 | 2 |
| **CLO-2** | 3 | 1 | 3 | 2 | 1 | 2 | 2 | 3 |
| **CLO-3** | 3 | 2 | 3 | 2 | 2 | 2 | 2 | 3 |
| **CLO-4** | 2 | 2 | 3 | 2 | 1 | 1 | 2 | 3 |
| **CLO-5** | 2 | 3 | 2 | 2 | 1 | 2 | 1 | 3 |

## Detailed Syllabus (CY451)

Perspectives, periodicity & periodic anomalies – Relativistic effects on chemical properties (2 h)

Hydrogen and its compounds: H-bond and its influence on the structure and properties of crystals- Hydrides→classification: electron deficient, electron precise and electron rich hydrides (2 h)

Alkali and alkaline earth metals: Solutions in liquid ammonia - Synthesis, properties, uses and structures of crown ether complexes, cryptands and organometallic compounds (2 h)

Group 13 elements: Borides, borates, boron halides, boranes, carboranes and metallocarboranes, BN compounds, transition-metal stabilized borylene and boryllithium, organoaluminum compounds, Lewis Base adducts of AlR3 compounds, Subvalent organo-Al compounds, Organo-gallium, -indium, and –thallium compounds (8 h)

Group 14 elements: Allotropes of Carbon- C60 and its compounds (fullerenes) - carbon nanotubes: synthesis and properties -Intercalation compounds of graphite - Pure Silicon, silica and silicates, Silicones - Low coordinated and hypervalent Silicon compounds - Brief survey of Ge, Sn, and Pb chemistry- Organo-germanium, -tin, and -lead compounds (6 h)

Group 15 elements: P(V) compounds (structure, bonding, reactivity) - P(III) compounds: diphosphenes, phosphaalkenes, iminophosphanes - P-containing ring systems (phosphabenzene, phosphole), phosphazenes, P-S compounds (7 h)

Group 16 elements: Sulfur - polycationic and anionic species - SN compounds.(3 h)

Group 17 elements: Charge-transfer complexes of halogens, interhalogen compounds, halogen oxides and oxygen fluorides, pseudohalogens. (3 h)

Group 18 elements: Noble gas clathrates and compounds. (3 h)

Inner transition elements: Chemistry of f-block elements - Binary compounds - Organometallic compounds - Relation to p-block and d-block chemistry - Transactinides (super-heavy elements). (4 h)

**Suggested reading:**

(1) A. G. Massey, "Main group chemistry", Wiley, 2000.
(2) N. N. Greenwood and A. Earnshaw, "Chemistry of the Elements", Pergamon Press, 1989.
(3) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Edn, OUP, 1999.
(4) C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(5) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Edn Wiley, 1999).
(6) J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Edn, Prentice Hall, 1997 (or a previous edition).

**Course Code : CY452**
**Title of the Course : Organic Reactions and Mechanisms**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** Basic and physical organic chemistry

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of reaction intermediates

**CLO-2 :** understand the insights of the reaction mechanism.

**CLO-3 :** understand the oxidation and reduction of organic chemistry.

**CLO-4 :** understand the detailed photochemical reactions and cyclization process.

**CLO-5 :** understand the impact of heterocycles in organic synthesis.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 3 |
| **CLO-2** | 3 | 2 | 3 | 2 | 3 | 2 | 2 | 3 |
| **CLO-3** | 3 | 3 | 2 | 2 | 2 | 3 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 3 | 3 | 3 | 3 |

## Detailed syllabus (CY452)

Methods of formation, structure determination and reactions of the following reactive intermediates: carbocations, carbanions, free radicals, carbenes and nitrenes, arynes and related species. [5 h]

Detailed reaction mechanisms and effect of different parameters in the regio-, stereo-, chemo-selective outcome of addition, substitution, elimination, oxidation, reduction, rearrangement and pericyclic reactions. [22 h]

Baldwin ring closure rules, formation of 3,4,5 and 6 membered rings. [2 h]

Reactions of aromatic heterocycles: Synthesis and properties. [4 h]

Organic photochemical reactions. [3 h]

**Suggested Text Books:**


1. M. B. Smith and J. March, March Advanced Organic Chemistry, 6$^{th}$ edition, Wiley, 2007.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5$^{th}$ Edition, Springer, 2007.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1$^{st}$ edition, Oxford University Press, 2001.
4. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company, 1999.
5. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6$^{th}$ edition, Pearson Education.
6. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. J. D. Coyle, Introduction to Organic Photochemistry, Wiley, 1991.
8. B. Halton, J. M. Coxon, Organic Photochemistry, Cambridge University Press, 2011.
9. S. Sankararaman, Pericyclic Reactions: A Textbook: Reactions, Applications and Theory, Wiley-VCH, 2005.

**Course Code : CY453**
**Title of the Course : Molecular Spectroscopy**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY404, CY403

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basic principles of light-matter interactions and learn quantum mechanical methods to analyze the interactions

**CLO-2 :** apply quantum mechanical methods to obtain selection rules and spectra of di- and poly-atomic molecules in microwave, infrared, Raman, UV-Vis spectroscopy

**CLO-3 :** learn various spectroscopic methods based on the magnetic resonance principles

**CLO-4 :** analyze spectroscopic information to obtain structural information of molecules

**CLO-5 :** learn principles of XPS and EPR spectroscopy to analyze the elemental composition, chemical bonding characteristics and radical nature of a sample

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 2 | 1 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 3 | 2 | 1 | 3 |

**Detailed Syllabus (CY453)**

Interaction of radiation with matter, semiclassical treatment. Time-dependent perturbation theory and transition rates. Electric dipole, quadrupole and magnetic dipole transitions. Selection rules. Line width and line shapes.

Rotational, vibrational and ro-vibrational spectroscopy of di-atomic molecules. Selection rules. Rotational energy levels of polyatomic molecules. Classification of rotors and selection rules. Applications. Polyatomic molecular vibrations. Local and normal modes. Infrared spectroscopy, selection rules. Rotational and vibrational Raman Spectroscopy and selection rules.

Franck-Condon principle. Electronic spectroscopy. Selection rules. Resonance Raman transitions and application. Radiative and nonradiative decay- internal conversion and intersystem crossing. Principles of Laser.

Electron Spectroscopy- PES, XPS and ESCA.

NMR spectroscopy-origin of chemical shift and spin-spin coupling. AX, AX2 and AXn systems. Paramagnetic shifts and their applications. Introduction to relaxation processes in solution.

EPR spectroscopy-relaxation processes. Origin of g-shifts and hyperfine coupling. Negative spin densities. Experimental determination of g, A and D tensors-their interpretation with examples.

Principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s.

**Suggested reading:**


1. Molecular Spectroscopy. I. N. Levine, Wiley –Interscience Publication.
2. Molecular Spectroscopy. J. D. Graybeal,McGraw Hill.
3. Modern Spectroscopy. J. M. Hollas, John Wiley & Sons.
4. High Resolution Spectroscopy. J. M. Hollas, Butterworths.
5. Fundamentals of Molecular Spectroscopy. C. N. Banwell and E. M. McCash, Tata McGraw-Hill publishing.
6. Principles of Ultraviolet Photoelectron Spectroscopy, J. W. Rabalais, John Wiley & Sons.
7. Molecular Spectra & Molecular Structure. G. Herzberg, Van Nostrand Reinhold Company.

**Course Code : CY454**
**Title of the Course : Chemical and Statistical Thermodynamics**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY404, CY151, CY403

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** discuss the principles of energy conservation, direction of flow of energy and direction of chemical reactions

**CLO-2 :** comprehend the concepts disorderedness in connection to the equilibrium properties of the system

**CLO-3 : a**ppreciate and develop the tools of statistical mechanics to systems under different conditions

**CLO-4 :** analyze of the connection of microscopic details of constituent molecules to the macroscopic properties of a system

**CLO-5 :** apply of tools and methods of equilibrium statistical mechanics to understand and analyze various properties of chemical systems

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 3 | 2 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 3 | 2 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 3 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 2 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 2 | 3 | 2 | 3 |

**Detailed Syllabus (CY454)**

Review of classical thermodynamics. Mathematical apparatus.

Concepts of statistical thermodynamics. Micro canonical, canonical and grand canonical ensembles. Ensemble averages. Most probable distribution. Undetermined multipliers. Fluctuations.

Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics.

Ideal monatomic, diatomic and polyatomic gas. Partition functions.

Equilibrium constant in terms of partition functions, Debye-Hückel theory. Statistical mechanics of ionic solutions. Flory-Higgins theory of polymer solutions. Specific heats of solids- Einstein and Debye models.

Virial equation of state and virial coefficients. The law of corresponding states. Elementary kinetic theory of transport in gases.

**Suggested reading**:

1. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
2. Physical Chemistry. I. N. Levine, McGraw Hill.
3. Physical Chemistry. R. G. Mortimer, Academic Press.
4. Statistical Mechanics. D. A. McQuarrie, University Science Books.

**Course Code : CY455**
**Title of the Course : Biological Chemistry**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** None

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to …**

**CLO-1 :** identify various classes of biomacromolecules and their building blocks

**CLO-2 :** appreciate the basic principles that govern the three-dimensional structures adopted by different classes of biomolecules

**CLO-3 :** understand the flow of information from genetic material to proteins and other biomolecules

**CLO-4 :** derive structure-function correlations for various classes of biomolecules

**CLO-5 :** appreciate that metabolic pathways which regulate biological processes basically involve chemical reactions mediated by enzymes and other biomolecules

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 1 | 2 | 2 | 1 | 1 | 1 | 3 |
| **CLO-2** | 3 | 2 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |

## Detailed Syllabus (CY455)

Cell Structure and Function: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells.

Introduction to biomolecules: Examples of biomolecules and building blocks of biopolymers. Types of reactions occurring in cells, structure of ice and liquid water, hydrogen bonding and hydrophobic interactions, buffers and the Henderson-Hasselbalch equation.

Amino acids, peptides and proteins: Primary structure of proteins, end group determination, amino acid analysis and the Edman degradation (protein sequencing), Ramachandran plot and the secondary structure of proteins α-helix, β-pleated sheet, β-bend and collagen triple helix. Tertiary structure and structural motifs - protein folding and domain structure of proteins. Oligomeric proteins. Purification and characterization of proteins, functions of proteins.

Enzymes and catalysis: Substrate specificity of enzymes, requirement of coenzymes, regulation of enzyme activity and allosteric effect, enzyme nomenclature, enzyme kinetics and the Michaelis-Menten equation, various types of enzyme inhibition. application of enzymes in chemical synthesis, enzyme models and their applications.

Nucleotides and nucleic acids: Ribonucleotides and deoxyribonucleotides, RNA and DNA. Base pairing, double helical structure of DNA and forces stabilizing nucleic acid structure. Methods used in nucleic acid separation and characterization, nucleic acid sequencing.

Transcription and translation: Messenger RNA, RNA polymerase and protein synthesis. Control of transcription and protein-DNA interactions. The genetic code, tRNA structure and codon-anticodon interactions. Ribosomes and their structure. Gene cloning and site-directed mutagenesis.

Carbohydrates: Monosaccharides, oligosaccharides and polysaccharides, carbohydrates of glycolipids and glycoproteins, role of sugars in biological recognition, blood group substances.

Lipids and membranes: Common classes of lipids - glycerolipids, phospholipids, sphingolipids and glycolipids. Self-association of lipids - formation of micelles, reverse micelles and membranes, gel and liquid-crystalline phases. Lipid phase polymorphism - bilayer, hexagonal and cubic phases. Liposomes and their properties and applications. Biological membranes and the fluid mosaic model, current models of biological membranes, membrane proteins and their functions, membrane asymmetry.

Introduction to metabolism: Overview of metabolism, catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.

**Suggested reading:**

1. Biochemistry by *D. Voet & J. G. Voet*, 4th Edition (2010) Published by John Wiley (New York).
2. Lehninger's Principles of Biochemistry by *D. L Nelson & M. M. Cox*, 5th Edition (2008) Published by W. H. Freeman (New York) and CBS Publishers (New Delhi).
3. Biochemistry by *J. M. Berg, J. L. Tymoczko & L. Stryer*, 5th Edition (2002) Published by W. H. Freeman (New York).

**Course Code : CY456**
**Title of the Course : Inorganic Chemistry Lab: Synthesis**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 3

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1:** provide basic principles of inorganic synthesis

**CLO-2:** understand the strategies for synthesis of various types of inorganic compounds

**CLO-3:** analyze and interpret physical properties in relation to the structure of the compound

**CLO-4:** design and execute a strategy for synthesis of a given compound

**CLO-5:** to synthesize and characterize a new compound

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed syllabus (CY456)

Synthesis of a variety of Inorganic Compounds/Complexes of 3d metal ions, main group elements and rare earths by using common experimental techniques.

Introduction to various physical measurements (IR, UV-Vis, Mass, NMR, Magnetic susceptibility, EPR and X-ray diffraction) for characterization of the compounds.

Analysis and interpretation of the physical data of the compounds to determine their structures.

Study of the related literature.

Preparation of Scientific Reports.

**Course Code : CY501**
**Title of the Course : Spectroscopic Methods for Structure Elucidation**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** A course on Molecular Spectroscopy (Physical Aspects)

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of different spectroscopic techniques (UV, Mass, IR and NMR).

**CLO-2 :** understand specialized and advanced spectroscopic experiments for the structural elucidation of organic compounds.

**CLO-3 :** do structural elucidation of unknown organic compounds using combined spectral data.

**CLO-4 :** design different spectroscopic experiments to address the regio and stereo chemical outcome in products of an organic reaction.

**CLO-5 :** apply different spectroscopic techniques to address the day to day societal needs.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-2** | 3 | 2 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-3** | 3 | 3 | 2 | 2 | 1 | 3 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 3 | 3 | 3 | 3 |

## Detailed syllabus (CY501)

**NMR Spectroscopy:** **[16 h]**

$^{1}$H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift □, inductive and anisotropic effects on □, chemical structure correlations of □, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects, examples of AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. $^{13}$C NMR, introduction to FT technique, relaxation phenomena, NOE effects, $^{1}$H and $^{13}$C chemical shifts to structure correlations. Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems). 2D NMR spectroscopy. Multinuclear NMR.

**Electronic spectroscopy:** **[3 h]**

Basic principle, electronic transitions and application to structure elucidation.

**Polarimetry**: **[1 h]**

Optical rotatory dispersion and circular dichroism.

**Infrared Spectroscopy:** **[5 h]**

Organic functional group identification through IR spectroscopy.

**Mass spectrometry:** **[6 h]**

Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules.

**Structure elucidation problems using the above spectroscopic techniques**: **[6 h]**

**Suggested Text Books**:


5. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
6. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
7. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, McGraw Hill, 6th edition 2007.
8. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
9. H. Gunther, NMR Spectroscopy Wiley-VCH, 2013.
10. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.

**Course Code : CY502**
**Title of the Course : Advanced Organic Synthesis**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** M.Sc courses in I – II semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1:** understand different types and distinctive features of advanced organic reactions and reagents

**CLO-2:** understand the advanced concepts related to the structure and properties of various organic reagents, catalysts and compounds

**CLO-3:** understand and analyze the structure, reactivity and properties of pharmaceutical drugs to natural organic compounds

**CLO-4:** design new catalysts, new reactions and properties based on the fundamental insights received about the molecules

**CLO-5:** appreciate the advanced sustainable reactions and catalysts for revolutionary applications

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |

## Detailed Syllabus (CY502)

Synthetic analysis and Planning: Retrosynthetic analysis, synthetic equivalent, control of stereochemistry, linear, convergent and divergent syntheses. (4 h)

Use of protecting groups in multi-step synthesis: Different protection and deprotection methods. (3 h)

Modern synthetic methods involving various oxidizing, reducing agents, C-C bond forming reactions by alkylation, acylation, organometallic, radical, pericyclic reactions and rerrangements. Discussion of selected syntheses of natural products/bioactive molecules/organic materials. (24 h)

Organocataytic transformations and C-H activation reactions-selected examples. Solid phase organic synthesis. (3 h)

Atom economy, step economy and green chemistry and environmental aspects. (2 h)

**Suggested reading:**

1. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis-An Introduction*, W. H. Freeman and Company, 2006.

2. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, Part B, Fifth Edition, 2007

3. E. J. Corey and X. M. Cheng, *The Logics of Chemical Synthesis*, Wiley, 1989.

4. K. C. Nicolaou, *Classics in Total Synthesis*, Vol 1, 2 and 3.

5. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2nd edition, Wiley, 2008.

6. J. H. Fuhrhop, G. Li, *Organic Synthesis: Concepts and Methods*, 3rd edition, VCH, 1994.

7. W. Carruthers, *Some Methods of Organic Synthesis*, Cambridge University Press.

8. H. O. House, *Modern Synthetic Reactions*, Benjamin-Cummings Publishing Co. 1972.

**Course Code : CY503**
**Title of the Course : Project - 1**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc courses in I and II semesters

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand research problems.

**CLO-2 :** execute literature search on a research topic.

**CLO-3 :** design new experiments to address research problems.

**CLO-4 :** conduct experiments in a scientific way.

**CLO-5 :** analyze and interpret the results.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 2 | 2 | 3 | 3 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 3 | 3 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 3 | 3 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |

# Detailed Syllabus (CY503)

Each student is assigned to a faculty supervisor to carry out a research project. The student gets trained on the following aspects:

- Literature survey on the assigned research topic using standard search tools such as SciFinder.
- Learning presentation tools such as Powerpoint, ChemDraw etc…
- Developing scientific writing and presentation skills by writing a report and oral presentation on the assigned topic.

**Course Code : CY504**
**Title of the Course : Chemical Dynamics**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc courses in I and II semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the various kinetic parameters, their measurements and utilities

**CLO-2 :** obtain theoretical understanding of how chemical reactions take place.

**CLO-3 :** learn experimental techniques for measuring the kinetics of fast reactions, homogeneous and heterogeneous catalyzed reactions.

**CLO-4 :** appreciate the theoretical and experimental developments in molecular reaction dynamics

**CLO-5 :** obtain an understanding of various transport properties in gas and solution phase.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| **CLO-2** | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 |
| **CLO-3** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY504)

1. Review of basic concepts in kinetics
2. Fast reactions: experimental techniques
3. Theories of reaction rates
4. Unimolecular reactions
5. Reactions in solution: reactions between ions, diffusion-controlled reactions, electron transfer reactions
6. Composite reactions including photochemical reactions
7. Homogeneous and heterogeneous catalysis
8. Kinetic isotope effect
9. Molecular reaction dynamics
10. Transport properties: Diffusion, viscosity, thermal conductivity, ion transport, dynamic electrochemistry

**Suggested reading:**


5. Physical Chemistry: A Molecular Approach. D. A. McQuarrie and J. D. Simon, University Science books
6. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
7. Physical Chemistry. I. N. Levine, McGraw Hill.
8. Chemical Kinetics. K.J. Laidler, Pearson.
9. Chemical Kinetics and Reaction Dynamics, P.L. Houston, Dover Publications, 2006

**Course Code : CY505**
**Title of the Course : Chemical Binding**

**L-T-P** : L / ~~T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY404, CY403, CY453

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** acquire fundamental understanding of structure and bonding in chemistry

**CLO-2 :** learn fundamental principles and concepts that leads to different types of chemical bond

**CLO-3 :** develop concept of molecular orbitals and their experimental manifestation and concept of electronic state

**CLO-4 :** explain the chemical reactivity based on electronic structure of molecules

**CLO-5 :** interpret underlying phenomena at a molecular level in all branches of chemistry

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 1 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 1 | 2 | 2 | 3 |
| **CLO-3** | 3 | 2 | 2 | 3 | 1 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 1 | 2 | 1 | 3 |

## Detailed Syllabus (CY505)

The Born-Oppenheimer approximation. Electronic structure theory: MO and VB theories, application to H2+ and H2. MO and VB wavefunctions of polyatomic systems. Hückel pi-electron theory. Walsh diagram and molecular geometry.

Hartree-Fock theory, Brillouin conditation, Non-orthogonal basis and Roothaan equation, SCF method. Koopmann's theorem.

Post Hartree-Fock methods. Electron correlation. Basis sets.

Density functional theory and application.

**Suggested reading:**

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
2. Quantum Chemistry, D. A. McQuarrie, University Science Books.
3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
5. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
6. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

**Course Code : CY506**
**Title of the Course : Advanced Inorganic Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3– 0 – 0

**Prerequisite Course / Knowledge (If any):** Basic inorganic chemistry/spectroscopy courses

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the structure, bonding, reactivity including safe handling of various organometallic compounds

**CLO-2 :** understand and apply the various organometallic compounds for catalytic applications relevant to chemical and polymer industries.

**CLO-3:** interpret the structure and function of various elements in biological systems using X-ray diffraction, spectroscopy and magnetic measurement techniques.

**CLO-4 :** explain the function of various elements in biological systems.

**CLO-5 :** design and develop new organometallic and bio-inorganic model systems.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed syllabus (CY506)

Recent Advances in Main Group Chemistry: Low and hypervalent compounds – p(pi)-p(pi) bonding in heavier main group chemistry. (3 h)

Organometallic Chemistry: Complexes with pi-acceptor and sigma-donor ligands - 16 electron and 18 electron rules – Stability and Reactivity - Isolobal analogy - Structure and bonding - Agostic interaction. (8 h)

Homogeneous and Heterogeneous Catalysis: Hydrogenation, carbonylation, polymerization, Wacker oxidation and other reactions catalyzed by transition metal complexes. (5 h)

Metal Cluster Compounds: Metal-metal bond - Carbonyl and non-carbonyl clusters - Structure and bonding - Low-dimensional solids - Clusters in catalysis. (4 h)

Bioinorganic Chemistry: Biochemistry of iron– its storage, transport and function; Transport and storage of dioxygen– structure and function of haemoglobin, myoglobin, hemocyanin and hemerythrin; Electron transport proteins– cytochromes and Fe-S proteins; Copper containing enzymes– blue and non-blue copper enzymes, ascorbate oxidase, tyrosynase, galactose oxidase, superoxide dismutase; Zinc containing enzymes– carboxy peptidase A, carbonic anhydrase, alcohol dehydrogenase; Iron containing enzymes– catalase, peroxidase and cytochrome P-450; Photosynthesis; Nitrogen fixation; Bioinorganic chemistry of alkali and alkaline earth metal cations; Toxicity of metals. (16 h) Inorganic Photochemistry: Ligand field photochemistry of $d^n$ complexes - Photochemistry of carbonyl compounds - Energy conversion (solar) and photodecomposition of water. (4 h)

**Suggested reading:**

(1) Textbooks suggested for CY-401.

(2) B. D. Gupta, A. J. Elias, "Basic Organometallic Chemistry", University Press, 2010.

(3) I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, "Bioinorganic Chemistry", VLSE with Univ. Sci. Books, 1998

(4) G. L. Miessler, D. A. Tarr, ''Inorganic Chemistry'', 3rd Edn, Pearson Education, 2004.

**Course Code : CY507**
**Title of the Course : Computer Applications and Programing Lab**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 3

**Prerequisite Course / Knowledge (If any):** A course on basic physics

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to**

**CLO-1:** understand electronic circuits used in spectrometers and research equipment

**CLO-2 :** have a theoretical and analytical understanding of how spectrometers and research equipment work

**CLO-3:** carry out minor repair of instruments

**CLO-4 :** design and fabricate minor equipment for research and analysis

### Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 2 | 2 | 2 | 2 | 2 | 1 | 1 | 2 |
| **CLO-2** | 2 | 2 | 2 | 2 | 3 | 1 | 1 | 2 |
| **CLO-3** | 2 | 2 | 2 | 2 | 3 | 1 | 2 | 2 |
| **CLO-4** | 2 | 2 | 2 | 2 | 2 | 1 | 1 | 2 |

## Detailed Syllabus (CY507)

C1 - Study of normal modes- optimization of molecular geometry, computation of normal modes and frequencies, analysis of the symmetries of the normal modes, effect of molecular symmetry on the degeneracies, impact of mass on the frequencies
C2 - Determination of equilibrium constants- optimization of molecular geometry of reactant and product, computation of the rotational constants, vibrational frequencies etc., calculation of partition functions, calculation of equilibrium constant at different temperatures
C3 - Determination of rate constants- optimization of molecular geometry of reactant and product, calculation of transition state, computation of the rotational constants, vibrational frequencies etc. for the reactant and transition state, calculation of partition functions, calculation of rates at different temperatures
C4 - Franck-Condon spectral calculations- optimization of the geometry of the ground, excited and ionized excited states, calculation of the vibrational frequencies of these states, calculation of the transition energies and oscillator strengths for the photo-electron spectra
C5 - Construction of Walsh diagram- computation of the MO energies at different geometries of a molecule (eg. H2O, Li2O), examination of the molecular orbitals and their symmetries, plot of the MO energies versus the geometric parameter reactant, qualitative analysis of the trends in the orbital energy variations
C6 - Woodward – Hoffman correlation diagrams- optimization of the geometries of cyclobutene and butadiene, computation of the molecular orbitals and their energies as a function of ring opening of cyclobutene under con- and dis-rotatory modes, plot of the frontier MO energies vs the ring opening coordinate (maintenance of symmetry), analysis of the plots and discussion about thermal / photochemical processes
C7 - Molecular modeling- H-bonded complexes – geometry optimization, analysis of energetics; exciton coupling in chromophore aggregates; effects of solvation
Alternative experiments- Intrinsic reaction coordinate, Natural bond orbital analysis

**Course Code : CY551**
**Title of the Course : Chemistry of Materials**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc courses in the I – III semesters

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** provide insight into the various classes and distinct features of materials

**CLO-2 :** appreciate the basic concepts related to the structure and properties of materials

**CLO-3 :** understand and analyze the structure-function correlations in materials

**CLO-4 :** design new materials based on a fundamental understanding of their attributes

**CLO-5 :** appreciate advanced materials for contemporary and futuristic applications

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY551)

**SOLID STATE STRUCTURE [5 h]**

Order - spatial, orientational; Types of solids; Symmetry in crystals - primitive lattice vector – Wigner-Seitz cell - crystal systems - Bravais lattices - crystallographic point groups and space groups; X-ray diffraction - reciprocal lattice - Ewald construction - structure factor - systematic absences - crystal structure solution and refinement - common crystal structure motifs; idea of quasicrystals.

**DEFECTS AND NONSTOICHIOMETRY [2 h]**

Point, line and plane defects; Intrinsic and extrinsic defects - vacancies, Schottky and Frenkel defects - charge compensation; Nonstoichiometry and defects - thermodynamic and structural aspects; Color centres.

**THERMAL PROPERTIES [2 h]**

Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conductivity.

**ELECTRICAL PROPERTIES [9 h]**

Free electron theory - electrical conductivity and Ohm's law - Hall effect; Band theory - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; Semiconductor/metal transition; p-n junctions; Superconductors - Meissner effect - type I and II superconductors - isotope effect - basic concepts of BCS theory - manifestations of the energy gap - Josephson devices.

**MAGNETIC PROPERTIES [3 h]**

Classification of magnetic materials; Langevin diamagnetism; Quantum theory of paramagnetism; Cooperative phenomena - ferro, antiferro and ferrimagnetism - magnetic domains and hysteresis; Superparamagnetism.

**OPTICAL PROPERTIES [2 h]**

Optical reflectance - plasmon frequency; Raman scattering in crystals; Photoconduction; Photo and electroluminescence; Lasers; Photovoltaic and photoelectrochemical effects.

**GENERAL CONCEPTS IN MATERIALS SYNTHESIS [3 h]**

Phase diagrams; Preparation of pure materials; Nucleation and crystal growth; Crystal growth techniques; Zone refining.

**INTRODUCTON TO DIFFERENT CLASSES OF MATERIALS [14 h]**

***HIGH $T_C$ MATERIALS***

Defect perovskites; High $T_C$ superconductivity in cuprates; Preparation and characterisation of 1-2-3 and 2-1-4 materials; Normal state properties - anisotropy; temperature dependence of electrical resistance - superconducting state; Applications.

***IONIC CONDUCTORS***

Types of ionic conductors; Mechanism of ionic conduction - interstitial jumps - vacancy mechanism – diffusion; Superionic conductors - phase transitions; Examples and applications of ionic conductors; Fuel cells.

***POLYMERS***

Molecular shape, structure and configuration; Crystallinity; Mechanical properties - stress-strain behaviour; Thermal behaviour - glass transition; Polymer types and their applications; Conducting, luminescent and ferroelectric polymers.

***LIQUID CRYSTALS***

Mesomorphic behaviour - thermotropic and lyotropic phases; Ordering in liquid crystals - the director field and order parameters; Nematic and smectic phases - phase transitions; Chiral nematics - cholesteric-nematic transition - optical properties - twisted nematic effect; Structure-phase relations.

***THIN FILMS***

Preparation techniques - evaporation/sputtering, chemical processes, MOCVD, sol-gel; Langmuir-Blodgett technique; Properties and applications of thin and ultrathin films.

***MOLECULAR MATERIALS***

Molecular semiconductors and metals; Organic superconductors; Molecular magnetic materials - single molecule magnets; Fullerenes - doped fullerene superconductors. Molecular electronics.

***NANOMATERIALS***

Preparation techniques; Scanning probe and electron microscopy; Novel physical phenomena in the nano domain – size effects; Electronic, photonic, magnetic and catalytic applications; Nanocomposites; Carbon nanotubes; Graphene; Molecular nanomaterials.

***NONLINEAR OPTICAL MATERIALS***

Nonlinear optical phenomena - second and third order effects; Molecular hyperpolarisability and second harmonic generation; Materials and structure-property correlations.

**Suggested Reading:**

1. H. V. Keer, Principles of the Solid State

2. L. E. Smart and E. A. Moore, Solid State Chemistry: an Introduction

3. M. T. Weller, Inorganic Materials Chemistry

4. K. J. Klabunde, Nanoscale Materials in Chemistry

5. W. D. Callister, Materials Science and Engineering, An Introduction

6. C. Kittel, Introduction to Solid State Physics

7. Journals like Chemistry of Materials, Journal of Materials Chemistry, Advanced Materials etc..

***Web resource:*** http://chemistry.uohyd.ac.in/~CY551/

**Course Code : CY552**

**Title of the Course : Project - II**

**L-T-P** : ~~L / T~~ / P
**Credits** : 0 – 0 – 9

**Prerequisite Course / Knowledge (If any):** None

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand research problems.

**CLO-2 :** execute literature search on a research topic.

**CLO-3 :** design new experiments to address research problems.

**CLO-4 :** conduct experiments in a scientific way.

**CLO-5 :** analyze and interpret the results.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 2 | 2 | 3 | 3 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 3 | 3 | 3 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 3 | 3 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY-552)

The student will continue to work in the same lab which was assigned for the Project-II in the previous semester.

The student will get trained in understanding research problem, addressing the chosen research problem by designing and executing experimental and/or computational experiments and analyse and interpret the results. At the end of the project each student will submit a report of the work done and make a presentation for evaluation.

**Course Code : CY571**
**Title of the Course : Organometallic Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** A course on understanding the basic principles of organometallic chemistry

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basics of main group chemistry (organolithium/ zinc/ magnesium/ copper/ titanium etc.)

**CLO-2 :** understand the insights of the organoboron, aluminium, and silicon chemistry.

**CLO-3 :** understand the chemistry of metal carbonyls/ carbenes/ benzynes/ NHC.

**CLO-4 :** understand the cross coupling reactions using Pd/Rh/Ru catalysts.

**CLO-5 :** understand the impact of C-H activations, Au-catalyzed transformations.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 3 |
| **CLO-2** | 3 | 2 | 3 | 2 | 3 | 2 | 2 | 3 |
| **CLO-3** | 3 | 3 | 2 | 2 | 2 | 3 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 3 | 3 | 3 | 3 |

## Detailed syllabus (CY571)

1) Organometallic Chemistry of Main Group and Transition metals for applications in organic transformations. [4 h]
2) Carbanionic Organometallics: Organolithium, magnesium, zinc , copper and titanium reagents. [4 h]
3) Chemistry of Organoboron, aluminium, silicon and tin compounds. [4 h]
   Organomercurials and organothalium compounds. [1 h]
4) Chemistry of Metal carbonyls: chromium, iron and cobalt carbonyl reagents. [2 h]
5) Metal carbon multiple bonds: carbenes, carbynes, and N-heterocyclic carbenes. [2 h]
6) Chemistry of Metallocenes: Ferrocene and related compounds. [2 h]
7) Organometallic Chemistry of the Noble Metal: Pd, Rh, Ru and Au catalyzed reactions, involving metal catalyzed coupling, C-H activation and metathesis reactions. [5 h]

**Suggested Text Books**:


1. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
2. J. F. Hartwig, Organotransition metal chemistry, University Science Books, 2010.
3. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4$^{th}$ edition, Wiley, 2005.
4. L. S. Hegedus, B. C. G. Söderberg, Transition Metals in the Synthesis of Complex Organic Molecules, University Science Books, 2010.

**Course Code : CY572**
**Title of the Course : Supramolecular Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 3 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc courses in the I – III semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** provide insight into the various supramolecular interactions

**CLO-2 :** appreciate the basis of supramolecular chemistry in terms of examples from nature

**CLO-3 :** understand and analyze the structure-function correlations from supramolecular perspective

**CLO-4 :** apply basic concepts of analytical and spectroscopic methods to understand host-guest chemistry

**CLO-5 :** apply Self-assembly and crystal engineering approach to understand host-guest chemistry

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 1 | 1 | 3 |
| **CLO-2** | 3 | 1 | 2 | 2 | 3 | 1 | 1 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 2 | 1 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |

## Detailed Syllabus (CY572)

**CONCEPTS** **[3 h]**

Definition, Development and Classification, Binding Constants, Supramolecular interactions

**SUPRAMOLECULAR CHEMISTRY IN LIFE** **[3 h]**

Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly

**CATION BINDING HOSTS** **[6 h]**

Podand, Crown Ether, Cryptand, Spherand - Nomenclature, Selectivity and Solution Behaviour. Alkalides, Electrides, Calixarenes, Siderophores

**ANION BINDING HOSTS** **[3 h]**

Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods

**ION PAIR RECEPTORS** **[2 h]**

Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction

**HOSTS FOR NEUTRAL GUEST** **[6 h]**

Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins

**CRYSTAL ENGINEERING** **[3 h]**

Concepts, Crystal Nucleation and Growth, Understanding Crystal Structures, Polymorphism, Co-crystals

**Suggested Reading:**


1) J. W. Steed & J. L. Atwood (2009), Supramolecular Chemistry, 2nd Edition, John Wiley
2) G.R. Desiraju (1989), Crystal Engineering. The Design of Organic Solids, Elsevier
3) G. R. Desiraju, J. J. Vittal, A. Ramanan (1989), Crystal Engineering -A Textbook, World Scientific-IISc Press
4) Recent papers from journals and reviews and monographs, etc

**Course Code : CY573**
**Title of the Course : Stereoselective Organic Synthesis**

**L-T-P** : L ~~/ T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY-452, CY-502 (or equivalent)

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1:** understand different types and distinctive features of advanced organic reactions, catalysts and reagents

**CLO-2:** understand the advanced concepts related to the structure and properties of various organic catalysts, reagents and compounds

**CLO-3:** understand and analyze the structure, reactivity and properties of catalysts, reagents, pharmaceutical drugs to natural organic compounds

**CLO-4:** design new catalysts, new reagents, new green reactions and properties based on the fundamental insights received

**CLO-5:** appreciate the advanced sustainable reactions, reagents and catalysts for revolutionary applications in modern chemical sciences

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |

## Detailed syllabus (CY573)

Brief review of stereochemistry (1 h)

Chiral pool approach, Acyclic stereoselection: reactions at α-and β–positions of a chiral center. Auxillary econtrolled stereoselection: Evans oxazolidones, Oppolzer sultams, Myers amides, Enders RAMP/SAMP, Shollkopf. (8 h)

Enantioselective alkylation allylation and crotylation reactions (2 h)

Asymmetric oxidation [epoxidation (Sharpless, Jacobsen, Shi), dihydroxylation (Sharpless)], reduction (Noyori, Corey, Pfaltz)
(3 h)

Organocatalyzed asymmetric synthesis (2 h)

Desymmetrization, Kinetic resolution reactions (3 h)

Application of the above methods in synthesis of selected biologically relevant molecules. (5 h)

**Suggested reading:**

1. M. Nogrady, *Stereoselective Synthesis: A Practical Approach*, Wiley, 2008.

2. E. M. Carreira, L. Kvaerno *Classics in Stereoselective Synthesis*, Wiley-VCH: Weinheim, Germany, 2009.

3. K. C. Nicolaou, E. J. Sorenson, *Classics in Total Synthesis*, Wiley-VCH.

4. K. C. Nicolaou, S. A. Snyder, *Classics in Total Synthesis II*, Wiley-VCH.

**Course Code : CY574**
**Title of the Course : Advanced Magnetic Resonance**

**L-T-P** : L / ~~T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** A course on Quantum Mechanics

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to**

**CLO-1:** understand the magnetic resonance phenomenon

**CLO-2 :** understand how multidimensional, multinuclear NMR work
**CLO-3:** design new (multidimensional) NMR experiments based on theoretical calculations

**CLO-4 :** cope up with the requirements for higher-level research on NMR spectroscopy

**CLO-5 :** seek a job as technician/operator in NMR labs

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 1 | 2 | 2 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 2 | 1 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 2 | 1 | 2 | 2 |

## Detailed Syllabus (CY574)

Review of electron and nuclear spins - angular momentum and magnetic moment: classical and quantum descriptions

Larmor precession, energy levels, and Bloch equation

Angular momentum operators of single and coupled spins: density matrix, unitary transformation, spin angular momentum product operators, spin Hamiltonians, transformations under the influence of rf and microwave pulses, coherence transfer

Spin Relaxation

Scalar and Dipolar interactions, Fermi contact and hyperfine interactions

Chemical shift, g-value, anisotropy

Effect of distortion of structure and symmetry on g-value

Molecular structure determination from J-coupling and NOE constraints

Magnetic field gradients, molecular diffusion, NMR and EPR imaging

**Suggested reading** :

R R Ernst, G Bodenhausen, A Wokaun "Principles of Nuclear Magnetic Resonance in One and Two Dimensions" (Oxford Science)

**Course Code : CY575**

**Title of the Course : Density Functional Theory**

**L-T-P** : L ~~/ T / P~~
**Credits** : 2 – 0 – 0

**Prerequisites:** CY403 (or equivalent)

**Detailed Syllabus (CY575)**

Many-electron wave functions; electron distributions and densities.

The Thomas-Fermi and Hartree-Fock Model. Slater Exchange Approximation.

The Hohenberg–Kohn theorems and the Kohn–Sham (KS) approach.

The Exchange-Correlation Functional. The Local Density Approximation (LDA).

The Generalized Gradient Approximation (GGA).

Hybrid functionals and the meta-GGA approaches. The Random Phase Approximation (RPA).

Implementations of density functional theory.

**Course Code : CY576**
**Title of the Course : Computational Chemistry**

**L-T-P** : L / ~~T/ P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY403, CY404, CY453, CY454, CY504

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 : u**nderstand bulk chemical processes at a molecular level

**CLO-2 :** develop concept of potential energy surfaces and understand their implications on reaction mechanism

**CLO-3 :** understand the celebrated Arrhenius equation and to learn derive it based on molecular level processes

**CLO-4 :** appreciate theories of reaction dynamics and their connection to the bulk chemical kinetics

**CLO-5 :** understand the transition state and its real time probing using femtosecond laser

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 1 | 2 | 1 | 3 |
| **CLO-2** | 2 | 3 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-3** | 3 | 2 | 2 | 3 | 1 | 2 | 1 | 3 |
| **CLO-4** | 2 | 3 | 2 | 2 | 1 | 2 | 2 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 1 | 2 | 2 | 3 |

## Detailed Syllabus (CY576)

Gas Phase Dynamics: Molecular beam scattering, Review of potential energy surface.
Dynamics of Molecular Collisions: Quasi-classical and quantum dynamics, cross section and rate constant. Microscopic mechanism of selected chemical reactions. Roming atom mechanism.
Microscopic interpretation of Arrhenius parameters.
Introduction to condensed phase dynamics, Krammer's theory and solvent effects.
Microscopic reversibility and detailed balance.
Marcus theory of electron transfer.
Femtochemistry- spectroscopic probing of transition state and control of chemical reactivity.

**Suggested reading:**

1. Theories of Molecular Reaction Dynamics, N. E. Henriksen and F. Y. Hansen, Oxford University Press.

2. Molecular Reaction Dynamics, R. D. Levine, Cambridge University Press.

3. Molecular Reaction Dynamics and Chemical Reactivity, R. D. Levine and R. B. Bernstein, Oxford University Press.

4. Tutorials in Molecular Reaction Dynamics, Eds. M. Brouard and C. Vallance, RSC Publishing.

**Course Code : CY577**
**Title of the Course : Computational Chemistry**

**L-T-P** : L /T/ P
**Credits** : 1 – 0 –1

**Prerequisite Course / Knowledge (If any):** CY403, CY504

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** appreciate fundamental understanding of structure and bonding in chemistry on a practical perspectives

**CLO-2 :** appreciate that the theory of molecular quantum chemistry aid in deriving quantitative information on structure and properties

**CLO-3 :** learn practical tools to solve Hartree-Fock Equation and density functional theory equation

**CLO-4 :** learn improvement of basic method with various electron correlation methods

**CLO-5 :** carry out hand-on exercise to do quantum chemistry calculations with the state-of-the-art software

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 1 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 1 | 2 | 2 | 3 |
| **CLO-3** | 3 | 2 | 2 | 3 | 1 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-5** | 3 | 3 | 2 | 3 | 1 | 2 | 1 | 3 |

## Detailed Syllabus (CY577)

One hour lecture + two hours laboratory per week

Review of Electronic Structure Theory: Hartree-Fock, MP2, DFT and configuration interaction. Basis sets, convergence.

Geometry optimization, frequency calculation, location of transition state, intrinsic reaction coordinates, population analysis, natural bond orbital analysis, calculation of thermodynamic parameters.

Calculation of molecular excited electronic states.

Representative examples.

**Suggested reading:**

1. Quantum Chemistry, I. N. Levine, PHI Learning Private Limited.

2. Essentials of Computational Chemistry- Theories and Models, C. J. Cramer, John Wiley and Sons, Ltd.

3. Introduction to Computational Chemistry, F. Jensen, John Wiley and Sons, Ltd.

4. Computational Chemistry- a Practical Guide for Applying Techniques to Real-World Problems, D. C. Young, John Wiley and Sons, Ltd.

## Course Code : CY578
## Title of the Course : Physical Methods for Inorganic Chemistry

**L-T-P** : L / ~~T~~ / ~~P~~
**Credits** : 2 – 0 – 0

**Prerequisite:** M.Sc. Semesters 1-3 courses in inorganic chemistry

Electronic and Photoelectron Spectroscopy: Excitation and ejection of electrons- Core level and valence- electron level photoelectron spectroscopy- Valence excitation spectroscopy- - Electronic spectra of transition metal complexes (3 h)

Vibrational Spectroscopy: Applications to Inorganic systems- Raman Spectra (1.5 h)

NMR Spectroscopy- Time scale- Multinuclear and Organometallic NMR spectroscopy - More common spin-1/2 nuclei, 19F, 31P, 29Si, 119Sn, 195Pt - Quadrupolar nuclei, e.g. 6Li, 11B, 14N, 17O and their characteristics and applications- Relaxation - Fluxional Processes- NMR spectroscopy of paramagnetic compounds- Lanthanide shift reagents, Shiftless reagents- Multiple resonance (3 h)

ESR Spectroscopy – Hamiltonian, Zeeman interaction, g-tensor, g–spread, g-value anisotropy, hyperfine coupling, and hyperfine anisotropy - dipolar contributions spin densities; exchange coupling, zero-field splitting- magnetic anisotropy - liquid, powder and single crystal studies - Variable temperature techniques- Examples from bioinorganic, coordination compounds and clusters (4.5 h)

Magnetism- Overview - Curie and Curie-Weiss law – Super exchange mechanism, Heisenberg- Dirac-van Vleck (HDvV) operator – Bleaney Bowers model- Spin ladder - Magnetic Measurements, Mechanisms of magnetic coupling - coupling in dimers - Single molecule magnets – Quantum tunneling - magneto structural correlations- Examples: Cu dimers, Spin clusters of Mn, Fe, and Cr, Mixed valence species (3 h)

Mössbauer Spectroscopy- Principles- 57Fe - Isomer shift, quadrupole splitting, magnetic hyperfine splitting, selected applications in Fen+ systems, Fe-S systems- Bioinorganic systems, Carbonyl compounds (1.5 h)

Diffraction methods: Distinction among X-ray, neutron and electron diffraction techniques- Single crystals and interpretation of results from X-ray crystallography (1.5 h)

**Suggested readings:**

(1) E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural methods in Inorganic Chemistry, ELBS, (Blackwell), 1987.
(2) R. S. Drago, Physical Methods in Chemistry (Saunders publishing)
(3) R. A. Scott and C. M. Lukehart (Editors) Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, 2007 [also available as Encyclopedia of Inorganic Chemistry, 5

**Course Code : CY579**
**Title of the Course : Elementary Polymer Chemistry**

**L-T-P** : L ~~/ T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc courses in the I - III semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the macromolecules, polymerization

**CLO-2 :** provide insight into the various classes of polymers and their synthetic process

**CLO-3 :** understand and analyze polymer molecular weights and various physical properties

**CLO-4 :** apply the basic concept of polymers in designing useful polymer materials

**CLO-5 :** apply the polymers for advanced applications.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 1 | 1 | 2 |
| **CLO-3** | 3 | 3 | 3 | 2 | 3 | 1 | 1 | 2 |
| **CLO-4** | 3 | 3 | 3 | 3 | 2 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY579)

Definition: Polymer, monomer, repeat unit, polymerization- Classification: Polymers based on source and polymerizations-polymer composition and structure- Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names- Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers)- Effect of Polymer structure on their properties (3 h)

Polymer Synthesis: Step, chain and miscellaneous polymerizations- Kinetics of polymerization- Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization- Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers- State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc. (6 h)

Polymer characterization - Chemical analysis of polymers, spectroscopic methods-IR, NMR, ESR, X-Ray Diffraction analysis- Microscopy- light Microscopy, Electron Microscopy and Electron Diffraction, Scanning electron microscopy- Thermal analysis- DSC, TGA, DMA, Rheology, Physical testing; stress-strain properties in tension (4.5 h)

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimm plot) (3 h)

Physical State and Morphology: Crystalline and Amorphous state- Thermal transitions- Glass-Rubber transition - Mechanical properties– stress-strain behaviour - Elastomer, Fibers and Plastics (3 h)

Polymer Blend and Nanocomposites: Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements, Uses (1.5 h)

Application of Synthetic Polymers: Materials and Biological importance and uses. Nanomaterials, Conducting polymers, Polymers for Energy applications. Physical aspects of polymers (1.5 h)

**Suggested reading:**

1. L. H. Sperling, Introduction to Physical Polymer Science, Wiley (1986)
2. H.R. Allcock and F.W. Lampe, Contemporary Polymer Chemistry, Prentice Hall (1990)
3. George Odian, Principles of Polymerization, 4th Edn, John Wiley (2004)
4. M. P. Stevens, Polymer Chemistry: An Introduction (2nd Edn), Oxford University Press (1990)
5. F.W. Billmeyer, Jr., Textbook of Polymer Science (1984), paperback
6. Relevant topics from modern literature

**Course Code : CY580**
**Title of the Course : Natural Products and Medicinal Chemistry**

**L-T-P** : L / ~~T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** MSc courses in the I – III semesters

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** provide insight into natural products and medicinal chemistry

**CLO-2 :** appreciate the basic concepts related to natural products and medicinal chemistry

**CLO-3 :** apply the basic concepts of new natural products and medicinal compounds based on a fundamental understanding

**CLO-4 :** understand the synthesis of natural products and medicinal compounds

**CLO-5 :** apply different synthetic techniques for synthesis of natural products and medicinal compounds

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 3 |

## Detailed Syllabus (CY580)

Biosynthesis, total synthesis, structure elucidation and biological significance of selected natural products. (12 h)

Introduction to drug discovery: Sources of drugs-natural products, drugs from organic synthesis, drug discovery and development
(2 h)

Drug structure and biological activity-pharmaceutically important functional groups physicochemical properties of drugs, electronic effects, spatial properties of drugs Fate of drugs in the body-absorption, distribution, metabolism, and excretion. Chemistry of drug metabolism, modifications to decrease metabolism, prodrugs Molecular mechanism of drug action-drug targets, receptors, enzymes, nucleic acids, non-receptor targets
(5 h)

Chemistry of selected drug classes-pharmacodynamic, chemotherapeutic, antibacterial, antiviral, antineoplastic, cardio-vascular, CNS, antihistamine, diabetic, analgesic and antiinflammatory drugs.
(5 h)

**Suggested reading:**

1. K. C. Nicolaou, Classics in Total Synthesis, Vol 1, 2 and 3.
2. J. H. Fuhrhop, G. Li, Organic Synthesis: Concepts and Methods, 3rd edition, VCH, 1994.
3. J. Mann, Chemical Aspects of Biosynthesis, Oxford University Press, 1994.
4. R. B. Silverman, The Organic Chemistry of Drug Design and Action, 2nd edition, Elsevier, New York, 2004.
5. G. L. Patrick, An Introduction to Medicinal Chemistry-5, Oxford University Press, 2013.

**Course Code : CY581**
**Title of the Course : Introduction to High Energy Materials**

**L-T-P** : L / ~~T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** A course on undergraduate level physical and organic chemistry

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** understand the basic concepts related to the High Energy Materials (HEM)

**CLO-2 :** provide insight into the distinct characteristics of HEM

**CLO-3 :** understand and analyze the structure-property correlations in HEM

**CLO-4 :** characterization of HEM

**CLO-5 :** designing and applications of HEM

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 2 | 2 | 2 | 1 | 1 |
| **CLO-2** | 2 | 3 | 3 | 3 | 3 | 2 | 2 | 1 |
| **CLO-3** | 1 | 2 | 3 | 3 | 3 | 3 | 2 | 2 |
| **CLO-4** | 1 | 1 | 1 | 2 | 3 | 3 | 3 | 2 |
| **CLO-5** | 1 | 1 | 1 | 2 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY581)

**Brief review of thermodynamics** **[3 h]**
Laws of thermodynamics, Definition of heat, energy, internal energy, enthalpy, free energy and entropy. Relationship between ΔE and ΔH, Cp and Cv. Bond energy.

**Thermo chemistry** **[2 h]**
Standard enthalpy of formation, enthalpy changes in reactions, thermo chemical equations, heat of combustion, Hess Law, calculations of enthalpies for various types of reactions.

**Requirement for High Energy Materials (HEM)** **[5 h]**
Explanation for energy release using bond energy calculations, energy release with respect to heats of formation, heat of explosion, Density factor, oxygen balance.

**Power of HEM** **[2 h]**
Volume of gas and heat releases in an explosion, Pressure and temperature rise in an explosion reaction, explosive power and power index.

**Decomposition reactions** **[4 h]**
Decomposition products from explosion reactions: Kistiakowesky-Wilkinson rule, modified K-W rule, Springer-Robert rule, water-gas equilibrium, determination of composition of decomposition products using equilibrium chemistry.

**Characterization of HEM** **[4 h]**
Bomb calorimeter, Use of TG-DTA and DSC for determination of various energetic parameters of HEM.

**Classification of HEM** **[3 h]**
Classification based on chemical groups present, Activation energy required for initiation of HEM, Classification based on explosive power and energy required for initiation of HEM.

**Burning of HEM** **[2 h]**
Combustion, detonation and deflagration processes; propellants, explosives and pyrotechnics. Propellant and explosive compositions, fuel, oxidizers, binders, plasticizers, thermite mixture, and other ingredients.

**Designing of HEM** **[3 h]**
Synthesis of representative examples of HEM. Research directions, Specific applications of HEM

**Suggested Reading:**


1. Book: The Chemistry of Explosives, ISBN 0-85404-640-2, RSC Paperbacks 2004, Jacqueline Akhavan.
2. Book: Demystifying Explosives: Concepts in High Energy Materials, ISBN 978-0-12-801576-6, Elsevier 2015. S. Venugopalan , HEMRL, Pune, India
3. Book: Introduction to Physics and Chemistry of Combustion: Explosion, Flame, Detonation, ISBN 3540787593, Springer 2008, Liberman Michael.

**Course Code : CY582**

**Title of the Course : Molecules and Materials for Electricity Production and Storage**

**L-T-P** : L / ~~T / P~~
**Credits** : 2 – 0 – 0

**Prerequisites:** None

**Molecules and Materials for Electricity Storage Devices:** Primary and secondary batteries and their working principles, electrode reactions, Inorganic and Organic Materials for anodes, cathodes and for transport of electrons and ions. Liquid and solid electrolytes used in the batteries.

**Molecules and Materials for Renewable Electricity Harvesting Devices:** Photovoltaic effect. Various types of solar cells and their operating principles. Inorganic and Organic Semiconductors, electron transport and hole transport in solar cells, efficiency of the solar cells and energy payback time.

**Course Code : CY583**
**Title of the Course : C-H functionalization**

**L-T-P** : L / ~~T / P~~
**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** CY-402, CY-452, CY-502

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students are expected to……**

**CLO-1**: understand and learn the origin and multidirectional growth, concept/philosophy of C-H functionalization process in synthetic chemistry.

**CLO-2:** understand significant contributions of scientists who developed the concept of C-H functionalization processes in synthetic chemistry and the way in which they surmounted the problems/difficulties in the course of development of concept and philosophy of C-H functionalization processes.

**CLO-3:** understand and appreciate the importance and high level applicability of C-H functionalization process in synthetic chemistry for obtaining enantiomerically enriched /pure compounds as well as for synthesis of natural products and bioactive molecules.

**CLO-4:** understand, learn, and address the difficulties in the applications of C-H functionalization processes in advanced synthetic strategies.

**CLO-5:** have developed an interest in the subject and the ability to invent/design novel strategies for C-H functionalization processes that will be useful to industries.

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | **2** |
| **CLO-4** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | **2** |
| **CLO-5** | 3 | 3 | 3 | 2 | 3 | 3 | 2 | 2 |

## Detailed Syllabus (CY583)

1) Origin and earlier reports: Concept and classification of C-H functionalization, C-H functionalization of acidic C-H bonds, C-H functionalization of less acidic C-H bonds

2) Friedel-Crafts reaction, intramolecular Friedel-Crafts reaction, asymmetric intramolecular Friedel-Crafts reaction, application to synthesis of natural products and bioactive compounds
3) Free radical mediated C-H functionalization reactions, Breslow remote functionalization and applications, other reactions
4) Fujiwara–Moritani reaction, Heck reaction including asymmetric Heck reaction, intramolecular Heck reaction, asymmetric intramolecular Heck reaction, application to synthesis of natural products and bioactive compounds, Catellani reaction
5) Baylis-Hillman reaction, asymmetric Baylis-Hillman reaction, intramolecular Baylis-Hillman reaction, asymmetric intramolecular Baylis-Hillman reaction, application to synthesis of natural products and bioactive compounds
6) C-H functionalization *via* C-H activation, origin of C-H bond activation and earlier reports, development of concept of C-H functionalization *via* C-H activation, asymmetric C-H functionalization *via* C-H activation, intramolecular version, asymmetric intramolecular version, application to synthesis of natural products and bioactive compounds
7) Miscellaneous reactions

**References**

**Books:** (1) Smith, M. B. March, J. J. *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th ed.; Wiley: New York, 2013**.** (2) Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry*; *Part A & B*, 5th ed.; Springer: New York, 2007. (3) Mundy, B. P ; Ellerd, M. G. ; Favaloro, F. G. *Name Reactions and Reagents in Organic synthesis* (2005) second edition John-Wiley and Sons Inc. New Jersey.

**Reviews:** (1) Rueping, M.; Nachtsheim, B. J. A review of new developments in the Friedel–Crafts alkylation–from green chemistry to asymmetric catalysis. *Beilstein J. Org. Chem.* **2010**, *6*, 6. doi:10.3762/bjoc.6.6. (2) Breslow, R. Biomimetic control of chemical selectivity. *Acc. Chem. Res.* **1980***, 13*, 170-177. (3) Mc Cartney, D.; Guiry, P.J. The asymmetric Heck and related reactions. *Chem. Soc. Rev.* **2011,** *40*, 5122–5150. (4) Beletskaya, I. P.; Cheprakov, A. V. The Heck reaction as a sharpening stone of palladium catalysis. *Chem. Rev.* **2000**, *100*, 3009-3066 (5) Basavaiah, D.; Veeraraghavaiah, G. The Baylis-Hillman reaction: A novel concept for creativity in chemistry. *Chem. Soc. Rev.* **2012**, *41*, 68-78. (6) Basavaiah, D., Reddy, B. S.; Badsara, S. S. Recent contributions from the Baylis-Hillman reaction to organic chemistry. *Chem. Rev.* **2010**, *110,* 5447–5674. (7) Gandeepan, P.; Müller, T.; Zell, D.; Cera, G.; Warratz, S.; Ackermann, L. 3d Transition metals for C−H activation. *Chem. Rev.* **2019**, *119,* 2192–2452. (8) Abrams, D. J.; Provencher, P. A.; Sorensen, E. J. Recent applications of C–H functionalization in complex natural product synthesis. *Chem. Soc. Rev.* **2018***, 47,* 8925−8967. (9) Wencel-Delord, J.; Glorius, F. C–H bond activation enables the rapid construction and late-stage diversification of functional molecules. *Nat. Chem.* **2013**, *5,* 369–375.

**Course Code : CY584**
**Title of the Course : Flow Chemistry and Process Intensification**

**L-T-P** : L / ~~T / P~~ Lectures only

**Credits** : 2 – 0 – 0 (2 lectures per week of 1 hour each)

**Prerequisite Course / Knowledge (If any)**: M.Sc. courses up to 3rd year of Integrated 5 year MSc / B.Sc. degree courses for 2 year M.Sc.

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to**

**CLO-1** : Understand the principles, equations and parameters required to convert reactions from batch to flow

**CLO-2** : Analyze and evaluate different types of reactions where flow chemistry has been successfully implemented

**CLO-3** : Select configurations for optimal process intensification from different types of flow reactors assembly

**CLO-4** : Understand the about design parameters for solid-solid, solid-liquid, liquid-liquid, and gas-liquid flow chemistry reactions

**CLO-5** : Assess the safety precautions and reactor size for different types of chemical processes in flow

**CLO 6** : Know about applications of drug and agro molecules for which flow process have been successfully optimized on manufacturing scale

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs) and Program Specific Outcomes (PSOs)**

| | PLO-1 | PLO-2 | PLO-3 | PLO-4 | PLO-5 | PLO-6 | PLO-7 | PLO-8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 3 | 3 | 3 | 3 | 2 | 3 | 3 |
| **CLO-2** | 3 | 3 | 3 | 3 | 3 | 2 | 3 | 3 |
| **CLO-3** | 3 | 3 | 3 | 3 | 3 | 2 | 3 | 3 |
| **CLO-4** | 3 | 3 | 3 | 3 | 3 | 2 | 3 | 3 |
| **CLO-5** | 3 | 3 | 3 | 3 | 3 | 2 | 3 | 3 |

### Detailed syllabus (CY584)

Introduction to flow chemistry and its advantages (2)

Recapitulate basic concepts of physical chemistry and reaction kinetics (2)

Principles and equations of flow chemistry (3)

Heterogeneous catalysis in flow chemistry reactions (4)

Pharmaceutical synthesis in flow reactors (5)

Different types of flow reactors (2)

Hazardous batch reactions done with ease in flow (3)

Handling of solids, liquids and gases reactants in flow (2)

Manufacture of Entresto/ commercial drugs in flow chemistry process (2)

Crystallization of polymorphs, cocrystals and salts in flow mode (4)

Important safety aspects essential in flow chemistry (2)

Video illustration of flow reactions (1)

Lectures by eminent academics covering recent research (3)

Brainstorming on design / development of batch to flow reactions by students (2)

**Suggested Reading**

1. Masuda et al. Flow fine synthesis with heterogeneous catalysts. Tetrahedron 2018, 74, 1705-1730.
2. Domokos et al. Integrated Continuous Pharmaceutical Technologies-A Review. Org. Process Res. Dev. 2021, 25, 721-739.
3. Mascia et al. End-to-End Continuous Manufacturing of Pharmaceuticals: Integrated Synthesis, Purification, and Final Dosage Formation. Angew. Chem. Int. Ed. 2013, 52, 12359-12363.
4. Bedard et al. Science, 2018, 361, 1220-1225.
5. Plutschack et al. The Hitchhiker's Guide to Flow Chemistry. Chem. Rev. 2017, 117, 11796-11893.
6. Cole et al. Kilogram-scale prexasertib monolactate monohydrate synthesisvunder continuous-flow CGMP conditions. Science, 356, 2017, 1144-1150.
7. Drahl, C&EN, March 12, 2018, p. 12.
8. Thaisrovings et al. Development of an Organometallic Flow Chemistry Reaction at Pilot-Plant Scale for the Manufacture of Verubecestat. Org. Process Res. Devp. 2018, 22, 403-408.

9. Akwi & Watts, Continuous flow chemistry: where are we now? Recent applications, challenges and limitations. Chem. Commun. 2018,54, 13894-13928.

10. Kleinbeck et al. Application of Transition-Metal Catalysis, Biocatalysis, and Flow Chemistry as State-of-the-Art Technologies in the Synthesis of LCZ696. J. Org. Chem. 2020, 85, 11, 6844–6853.

11. Narala et al. Pharmaceutical Co-crystals, Salts, and Co-amorphous Systems: A novel opportunity of hot-melt extrusion. Journal of Drug Delivery Science and Technology, 2021, 61, 102209.

12. Gerardy & Monbaliu. Multistep Continuous-Flow Processes for the Preparation of Heterocyclic Active Pharmaceutical Ingredients. Top. Heterocycl. Chem. DOI: 10.1007/7081_2018_21.

13. Hartman, McMullen, Jensen. Deciding Whether To Go with the Flow: Evaluating the Merits of Flow Reactors for Synthesis. Angewandte Chemie International Edition, 2011, 50, 33, 7502-7519.

14. Gutmann, Cantillo, Oliver Kappe. Continuous-Flow Technology—A Tool for the Safe Manufacturing of Active Pharmaceutical Ingredients. Angewandte Chemie International Edition, 2015, 54, 23, 6688-6728.

15. Norbert Kockmann et al. Safety assessment in development and operation of modular continuous-flow processes. React. Chem. Eng., 2017, 2, 258-280.

**Web resource**: http://chemistry.uohyd.ac.in/~CY584/

**Course Code : CY585**
**Title of the Course : Introduction to Molecular Simulation Techniques**

**L-T-P : L ~~/ T / P~~**

**Credits** : 2 – 0 – 0

**Prerequisite Course / Knowledge (If any):** Quantum chemistry, Statistical thermodynamics and Fortran Programming

## Course Learning Outcomes (CLOs)

**After completion of this course successfully, the students will be able to……**

**CLO-1 :** Understand the basics of Statistical Mechanics

**CLO-2 :** Learn about empirical parameters to model interactions in classical simulations

**CLO-3 :** Learn basics of Monte Carlo Simulations and Molecular Dynamics Simulations

**CLO-3 :** Learn how to calculate dispersion and electrostatic interactions

**CLO-4 :** Apply Molecular Dynamics simulation techniques to understand structure of liquid

**CLO-5 :** Learn basics of Free energy calculations and Rare event simulation techniques

**CLO-6** : Apply Monte Carlo and Molecular Dynamics simulation techniques to realistic bulk systems

## Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs)

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 3 | 0 | 3 | 3 | 0 | 2 | 1 | 3 |
| **CLO-2** | 3 | 0 | 3 | 2 | 0 | 2 | 1 | 3 |
| **CLO-3** | 3 | 0 | 2 | 3 | 2 | 2 | 1 | 3 |
| **CLO-4** | 3 | 3 | 2 | 3 | 3 | 2 | 3 | 3 |
| **CLO-5** | 3 | 0 | 2 | 2 | 1 | 2 | 1 | 3 |
| **CLO-6** | 3 | 2 | 3 | 3 | 3 | 3 | 3 | 3 |

## Detailed Syllabus (CY585)

Classical Statistical Mechanics, Liouville operator, Ergodicity (3)

Ensembles, Fluctuations and Time Correlation Functions (2)

Introduction to Computer Simulations, Force fields, Periodic Boundary Conditions (2)

Monte Carlo Simulations; Importance Sampling and Metropolis Method (4)

Molecular Dynamics Simulations ( Verlet and Great Predictor-corrector algorithm, Neighbour List ) (4)

Long-range forces (Ewald Sum) (1)

Analysis of Liquid Structure (2)

Free energy estimation Methods (2)

Rare Event Simulations (1)

Applications: Melting, Protein-drug binding, Transport Properties of Liquids, (3) Adsorption Isotherms

## Suggested Reading:

1. Computer Simulation of Liquids by D. J. Tildesley and M.P. Allen

2. Understanding Molecular Simulation: From Algorithms to Applications by Berend Smit and Daan Frenkel

## Course Code : CY586

## Title of the Course : AI-ML and Blockchain in Chemistry (Elective Course for 2 Credits)

**L-T-P** : L / T / P
**Credits** : 1– 0 –1

**Prerequisite Course / Knowledge (If any):** Familiarity with any computer programming language and interest to learn new concepts and algorithms.

**Course Learning Outcomes (CLOs)**

**After completion of this course successfully, the students will be able to:**

**CLO-1 :** Learn a new Computer Programming Language, Python.

**CLO-2 :** The student would be introduced to the basics of artificial intelligence and hands-on experience using the python pprogramming language.

**CLO-3 :** Learn the basics of machine learning algorithms and use the same for solving scientific problems.

**CLO-4 :** Learn basics and types of deep learning and blockchain algorithms and develop programs in Python.

**CLO-5 :** Finally, the student would be able to apply and develop his/her own AI/ML-based computer programs.

**Mapping of Course Learning Outcomes (CLOs) with Program Learning Outcomes (PLOs) and Program Specific Outcomes (PSOs)**

| | PLO 1 | PLO 2 | PLO 3 | PLO 4 | PLO 5 | PLO 6 | PLO 7 | PLO 8 |
|---|---|---|---|---|---|---|---|---|
| **CLO-1** | 2 | 3 | 3 | 3 | 1 | 3 | 2 | 3 |
| **CLO-2** | 3 | 3 | 3 | 2 | 1 | 3 | 2 | 3 |
| **CLO-3** | 3 | 3 | 3 | 2 | 1 | 3 | 2 | 3 |
| **CLO-4** | 3 | 3 | 3 | 2 | 1 | 3 | 2 | 3 |
| **CLO-5** | 3 | 3 | 3 | 2 | 1 | 3 | 2 | 3 |

## Detailed Syllabus (CY586)s

1. **Introduction to Artificial intelligence, Machine Learning, Deep Learning and Blockchain Algorithms.**
2. **Python Programming Language:**
   - **2.1 Introduction to Python:** Basic structure of Python programs and Data Structures.
   - **2.2 Python for Data Science:** Two important libraries of Python – *NumPy* and *Pandas.*
   - **2.3 Mathematics for Machine Learning:** Linear Algebra, Matrices, Multi-Variable Calculus and Vectors.
   - **2.4 Data Visualization in Python:** Graphs plotting using Python.
   - **2.5 Basic and Data Analysis using SQL:** Basics of SQL.

3. **Basics of Machine Learning:** Basics of Machine Learning and algorithms.
   - **3.1 Linear Regression:** Basics of linear regression and applications in chemistry.
   - **3.2 Logistic Regression:** Multivariate Logistic Regression and Implementation in Python.

4. **Advanced Machine Learning:** ML models such as supervised and unsupervised algorithms.
   - **4.1 Advanced Regression:** Generalized Linear Regression and Regularized Regression techniques.
   - **4.2 Support Vector Machine:** SVM algorithm, its working, kernels and implementation.
   - **4.3 Tree Models:** Basics of Tree models, their structure, splitting techniques and pruning.
   - **4.4 Unsupervised Learning:** Clustering, its types, basics of PCA, its working and implementation in Python.

5. **Deep Learning:** Types of Neural Networks covered along with implementation.
   - **5.1 Neural Networks:** Basics of Neural Networks, activation functions, and Feed Forward network.
   - **5.2 Convolutional Neural Network (**CNN): CNN structure, layers, and working.
   - **5.3 Recurrent Neural Networks** (RNN)**:** RNN and LSTM with their implementations.

6. **Practical Hands-on Sci-Kit Learn and Keras/TensorFlow software packages.**

**Suggested reading:**


1. Bishop, C. M. (2006) Pattern Recognition and Machine Learning.
2. Goodfellow, I., Bengio, Y. and Courville, A. (2016) Deep Learning. MIT Press.
3. Bengio, Y., LeCun, Y., Hinton, G. (2015). Deep Learning. Nature 521: 436-44.
4. Stuart J. Russell and Peter Norvig, (2015) Artificial Intelligence: A Modern Approach, Pearson.
5. Schmidhuber, J. (2015) Deep Learning in Neural Networks: An Overview.
6. Aurélien Géron, (2019) Hands-On Machine Learning with Scikit-Learn and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems, O'Reilly.
7. ScikitLearn
8. Keras: https://keras.io/
9. TensorFlow: https://www.tensorflow.org/