

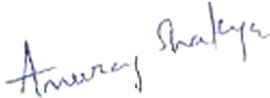
**MANGALAYATAN UNIVERSITY, ALIGARH**  
**CENTRE FOR DISTANCE AND ONLINE EDUCATION**



**PROGRAMME PROJECT REPORT**  
**MASTER OF SCIENCE (CHEMISTRY)**

**2025-26**

  
Registrar  
Mangalayatan University  
Beswan, Aligarh

  
Director  
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Mangalayatan University, Beswan, Aligarh-202146 (U.P.)

## **Introduction**

Master of Science in Chemistry (M.Sc. Chemistry) is a postgraduate programme that delves into advanced chemical concepts and theories. This programme is meticulously crafted to empower students with a profound comprehension of various chemical principles and their wide-ranging applications across various domains, including pharmaceuticals, materials science, environmental science, and chemical engineering. The comprehensive curriculum encompasses advanced topics such as quantum chemistry, chemical thermodynamics, spectroscopy, organic synthesis, and chemical kinetics, among others. Through M.Sc. Chemistry programme, students not only acquire theoretical knowledge but also gain practical laboratory skills, enabling them to conduct cutting-edge research and contribute to advancements in the field of chemistry.

M.Sc. Chemistry students are encouraged to engage in independent research projects and collaborative endeavours, fostering the development of vital teamwork and communication abilities. They are introduced to state-of-the-art laboratory techniques and modern analytical instruments, which strengthen their capacity for problem-solving. Moreover, this programme emphasizes the application of chemical knowledge in real-world scenarios, fostering the development of innovative solutions to complex challenges. Graduates of M.Sc. Chemistry programme emerge as highly skilled chemists, well-prepared to pursue careers in academia, research and development, pharmaceuticals, chemical manufacturing and various other sectors where a profound understanding of chemistry is indispensable. This rigorous and fulfilling programme offers students a solid foundation in chemistry, positioning them for a diverse array of exciting career prospects in the dynamic field of chemistry.

## **A. Programme's Mission and Objectives**

### **Mission**

- To cater and ensure excellent theoretical and practical training through teaching, counseling and mentoring with a view to achieve professional and academic excellence.
- To connect with industry and incorporating knowledge for research enhancement.
- To generate, disseminate and preserve knowledge for the benefit and betterment of society.

### **Objectives**

M.Sc. Chemistry programme has a comprehensive set of objectives aimed to providing students with a deep and advanced understanding of the field. It seeks to instill a strong foundation in core chemical principles and theories while promoting critical thinking and analytical skills. Additionally, the programme aims to cultivate students' ability to conduct independent research, including honing skills in literature review, experimental design, data analysis and effective scientific communication. It aligns curriculum with the evolving needs of industries and academia to ensure that graduates are well-prepared for diverse career opportunities, spanning academia, research, pharmaceuticals, environmental science, and various other sectors. Ultimately, the programme contributes to the advancement of scientific knowledge and innovation within the realm of chemistry.

## **B. Relevance of the Programme with HEI's Mission and Goals**

The vision and mission of HEI, Mangalayatan University, Aligarh, are:

### **Vision**

To be an institution where the most formative years of a young mind are spent in the guided pursuit of excellence while developing a spirit of inquisitive questioning, an ability to excel in the pressure of a fast-changing professional world, and a desire to grow into a personality rather than a person, in an environment that fosters strong moral and ethical values, teamwork, community service and environment consciousness.

### **Mission**

- To be the enablers of the confluence of academic rigor and professional practicality
- To bring global best practices to students through widespread use of technology.
- To empower our faculty to constantly develop new skills and excel professionally.

- To provide the best campus environment to students and faculty with all facilities to nurture their interest.

M.Sc. (Chemistry) programme of the University strives to realize its vision and mission by rectifying student centric issues on priority and also to empower local community with the help of various social clubs running in University like NSS, KADAM and Alumni association. The University promotes multidisciplinary and allied research in various fields that supports and harnesses joyful learning environment. The goals of ODL (Open Distance Learning) programme is to provide educational facilities to all qualified and willing persons who are unable to join regular courses due to personal or professional reasons. There are many potential learners who cannot afford to join regular courses due to professional responsibilities and personal commitments. For such cases M.Sc. (Chemistry) through ODL mode can be helpful in enhancing knowledge base and skill up-gradation.

The programme aims to provide alternative path to wider potential learners who are in need of refresher courses to update their skills.

#### **C. Nature of Prospective Target Group of Learners**

Distance Education of Mangalayatan University (MU) shall target the working professional's executives as well as those who cannot attend a full-time programme due to prior occupation or other assignments. The candidates desirous of taking admission in M.Sc. (Chemistry) programme shall have to meet the eligibility norms as follows-

1. *To obtain admission in M.Sc. (Chemistry) programme offered through ODL mode.*
2. *The learner must have completed graduation in science stream (PCM/ZBC).*

#### **D. Appropriateness of Programme to be conducted in ODL mode to acquire specific skills and competence**

The University has identified the following **Programme Outcomes** and **Programme Specific Outcomes** as acquisition of specific skills and competence in M.Sc. (Chemistry) Programme.

##### **Programme Outcomes (PO's)**

After completing the M.Sc. (Chemistry) programme through ODL Mode, students will be able to:

- a. PO1: Knowledge outcomes: Acquire knowledge and ability to develop creative solutions, and better understanding of the future developments of the subject. Also evolve analytical and logical thinking abilities.
- b. PO2: Skill Outcomes: Learn and understand the new concepts and get prepared for placement by developing scientific skills. Further ability to communicate scientific information in a clear and concise manner.
- c. PO3: General Competence: Be able to understand the role of science in solving real life problems and get an ability to participate in debates and discussions constructively.
- d. PO4: Scientific Aptitude and Innovation: Know the recent developments, future possibilities and able to gather, assess, and make use of new information and applying this knowledge to find creative solutions.

##### **Programme Specific Outcomes (PSO's)**

After completing the M.Sc. (Chemistry) programme through ODL Mode, students will be able to:

- a. PSO1: Students will understand the basic concepts, fundamental principles, and the scientific theories related to various scientific phenomena and their relevancies in the day-to-day life. They will also be able to acquire knowledge about the fundamentals and applications of chemical and scientific theories.
- b. PSO2: Helps in understanding the causes of environmental pollution and can open up new methods for environmental pollution control.

- c. PSO3: Students will become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental, polymer and biochemistry. They will also learn to apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.
- d. PSO4: Provide a systematic understanding of the concepts and theories of chemistry and their application in the real world – to an advanced level, and enhance career prospects in a huge array of fields.

**E. Instructional Design**

The programme is divided into four semesters and minimum credit requirement is 80 to get M.Sc. (Chemistry) degree in ODL mode from Mangalayatan University. Minimum time period for acquiring M.Sc. (Chemistry) degree will be two years and maximum time period to acquire is 4 years.

### Evaluation Scheme

| <b>Semester-I</b> |                    |                          |                 |               |                                    |                            |                    |
|-------------------|--------------------|--------------------------|-----------------|---------------|------------------------------------|----------------------------|--------------------|
| <b>S. No.</b>     | <b>Course Code</b> | <b>Course Name</b>       | <b>Category</b> | <b>Credit</b> | <b>Continuous Assessment Marks</b> | <b>Term End Exam Marks</b> | <b>Grand Total</b> |
|                   |                    |                          |                 |               | <b>Max. Marks</b>                  | <b>Max. Marks</b>          |                    |
| 1                 | CHM-6111           | Inorganic Chemistry – I  | DCC             | 4             | 30                                 | 70                         | 100                |
| 2                 | CHM-6112           | Organic Chemistry – I    | DCC             | 4             | 30                                 | 70                         | 100                |
| 3                 | CHM-6113           | Physical Chemistry - I   | DCC             | 4             | 30                                 | 70                         | 100                |
| 4                 | CHM-6114           | Analytical Chemistry – I | DCC             | 4             | 30                                 | 70                         | 100                |
| 5                 | CHM-6151           | Chemistry Lab - I        | DCC             | 2             | 30                                 | 70                         | 100                |
| 6                 | CHM-6152           | Chemistry Lab - II       | DCC             | 2             | 30                                 | 70                         | 100                |
| <b>Total</b>      |                    |                          |                 | <b>20</b>     | <b>180</b>                         | <b>420</b>                 | <b>600</b>         |

| <b>Semester-II</b> |                    |   |                 |               |                                    |                            |                    |
|--------------------|--------------------|---|-----------------|---------------|------------------------------------|----------------------------|--------------------|
| <b>S. No.</b>      | <b>Course Code</b> | <b>Course Name</b>                            | <b>Category</b> | <b>Credit</b> | <b>Continuous Assessment Marks</b> | <b>Term End Exam Marks</b> | <b>Grand Total</b> |
|                    |                    |   |                 |               | <b>Max. Marks</b>                  | <b>Max. Marks</b>          |                    |
| 1                  | CHM-6211           | Inorganic Chemistry – II                      | DCC             | 4             | 30                                 | 70                         | 100                |
| 2                  | CHM-6212           | Reactions and Mechanisms in Organic Chemistry | DCC             | 4             | 30                                 | 70                         | 100                |
| 3                  | CHM-6213           | Physical Chemistry - II                       | DCC             | 4             | 30                                 | 70                         | 100                |
| 4                  | CHM-6214           | Analytical Chemistry - II                     | DCC             | 4             | 30                                 | 70                         | 100                |
| 5                  | CHM-6251           | Chemistry Lab - III                           | DCC             | 2             | 30                                 | 70                         | 100                |
| 6                  | CHM-6252           | Chemistry Lab - IV                            | DCC             | 2             | 30                                 | 70                         | 100                |
| <b>Total</b>       |                    |   |                 | <b>20</b>     | <b>180</b>                         | <b>420</b>                 | <b>600</b>         |

| <b>Semester-III</b> |                    |  |                 |               |                                    |                            |                    |
|---------------------|--------------------|--|-----------------|---------------|------------------------------------|----------------------------|--------------------|
| <b>S. No.</b>       | <b>Course Code</b> | <b>Course Name</b>                           | <b>Category</b> | <b>Credit</b> | <b>Continuous Assessment Marks</b> | <b>Term End Exam Marks</b> | <b>Grand Total</b> |
|                     |                    |  |                 |               | <b>Max. Marks</b>                  | <b>Max. Marks</b>          |                    |
| 1                   | CHM-7111           | Biophysical and Computational Chemistry      | DCC             | 4             | 30                                 | 70                         | 100                |
| 2                   | CHM-7112           | Organometallic Chemistry                     | DCC             | 4             | 30                                 | 70                         | 100                |
| 3                   | CHM-7113           | Heterocyclic Chemistry and Organic Synthesis | DCC             | 4             | 30                                 | 70                         | 100                |
| 4                   | CHM-7114           | Research Methodology                         | GE              | 4             | 30                                 | 70                         | 100                |
| 5                   | CHM-7151           | Chemistry Lab – V                            | DCC             | 2             | 30                                 | 70                         | 100                |
| 6                   | CHM-7152           | Chemistry Lab – VI                           | DCC             | 2             | 30                                 | 70                         | 100                |
| <b>Total</b>        |                    |  |                 | <b>20</b>     | <b>180</b>                         | <b>420</b>                 | <b>600</b>         |

| <b>Semester-IV</b> |                                    |  |                 |               |                                    |                            |                    |
|--------------------|------------------------------------|--|-----------------|---------------|------------------------------------|----------------------------|--------------------|
| <b>S. No.</b>      | <b>Course Code</b>                 | <b>Course Name</b>                             | <b>Category</b> | <b>Credit</b> | <b>Continuous Assessment Marks</b> | <b>Term End Exam Marks</b> | <b>Grand Total</b> |
|                    |                                    |  |                 |               | <b>Max. Marks</b>                  | <b>Max. Marks</b>          |                    |
| 1                  | CHM-7211                           | Green Chemistry                                | DCC             | 2             | 30                                 | 70                         | 100                |
| 2                  |                                    | Elective -1                                    | Elective        | 4             | 30                                 | 70                         | 100                |
| 3                  |                                    | Elective -2                                    | Elective        | 4             | 30                                 | 70                         | 100                |
| 4                  | CHM-7251                           | Chemistry Lab - VII                            | DCC             | 2             | 30                                 | 70                         | 100                |
| 5                  | CHM-7252                           | Chemistry Lab - VIII                           | DCC             | 2             | 30                                 | 70                         | 100                |
| 6                  | CHM-7291/<br>CHM-7217+<br>CHM-7253 | Project/<br>(Environmental<br>Chemistry + Lab) | DCC             | 6/<br>(4+2)   | 0/(30+30)                          | 200/(70+70)                | 200                |
| <b>Total</b>       |                                    |  |                 | <b>20</b>     | <b>150/210</b>                     | <b>550/490</b>             | <b>700</b>         |

#### List of Elective Papers

|           |                              |          |
|-----------|------------------------------|----------|
| CHM-7212  | Supramolecular Chemistry     | Elective |
| CHM-7213  | Materials Chemistry          | Elective |
| CHM- 7214 | Chemistry of Natural Product | Elective |
| CHM- 7215 | Polymer Chemistry            | Elective |
| CHM-7216  | Medicinal Chemistry          | Elective |

#### Total credit of M.Sc. (Chemistry) programme semester wise

| <b>Semester</b> | <b>Credit</b> |
|-----------------|---------------|
| I               | 20            |
| II              | 20            |
| III             | 20            |
| IV              | 20            |
| <b>TOTAL</b>    | <b>80</b>     |

**MOOCs**

The University shall give flexibility in opting for MOOCs (Massive Online Open Courses) by the students pertaining to the prescribed curriculum and also the credits earned in the MOOCs may be dealt as part of the evaluation scheme as per UGC (Open and Distance Learning Programmes and Online Programmes) Regulations, 2020.

**Syllabi and Course Materials**

Syllabi, PPR and self-learning materials are developed mostly by experienced faculty members of Mangalayatan University in consultation with contents experts and the same will be forwarded to CIQA and BoS/Academic Council/ Executive Council for further suggestions and approval.

## SEMESTER: I

**Course Name: Inorganic Chemistry- I**

**Code: CHM-6111**

**Credits: 4**

### **Course Objectives**

This course aims to equip students with a robust understanding of bonding theories, coordination chemistry, and the structural diversity of inorganic compounds. Through exploring valence bond, crystal field, and molecular orbital theories, students will analyze bonding in main-group molecules, phosphorus-nitrogen/sulfur systems, and transition metal complexes. The curriculum emphasizes practical insights into alkali/alkaline earth metal coordination, catalytic applications, and metal cluster chemistry. Students will gain proficiency in predicting molecular geometries, stability trends, and reactivity patterns while connecting concepts to real-world applications in catalysis, environmental science, and industrial processes.

### **Block I: Structure and Bonding in Main Group Compounds**

#### **Unit 1: Bonding in Inorganic Molecules**

Various Theories of Bonding in Inorganic Molecules, Limitations and Applications - (VBT, CFT, and LFT), Hybridization.

#### **Unit 2: VSEPR Theory**

VSEPR, Walsh Diagram (Triatomic and Penta-Atomic Molecules),  $d\pi-p\pi$  Bond, Bent Rule and Energetic Of Hybridization, Some Simple Reactions of Covalently Bonded Molecules.

#### **Unit 3: Phosphorus-Nitrogen Compounds**

Synthesis, Structure, Bonding and Uses of Phosphorus-Nitrogen Compounds: Cyclo and Linear Phosphonitrilic Compounds.

#### **Unit 4: Phosphorus-Sulphur and Sulphur-Nitrogen Compounds**

Synthesis, Structure, Bonding and Uses of Phosphorus-Sulphur Compounds, Sulphur- Nitrogen Compounds, Ring and Chain Compounds  $S_2N_2$ ,  $S_4N_4$ .  $(SN)_x$  etc.

### **Block II: Alkali and Alkaline Earth Metal Complexes**

#### **Unit 5: Coordination Chemistry of Alkali and Alkaline Earth Metals**

General Properties and Coordination Behavior, Factors Affecting Coordination Number and Geometry, Common Ligands: Crown Ethers, Cryptands, Calixarenes, and their Selectivity for Alkali and Alkaline Earth Metals, Chelate Effect in Complexes of Alkali and Alkaline Earth Metals.

#### **Unit 6: Structure and Stability**

Mononuclear, Polynuclear, and Cluster Complexes, Thermodynamic Stability Constants: Stepwise and Overall Stability of Complexes, Role of Hard and Soft Acids and Bases (HSAB) Theory in Predicting Stability, Influence of the Size, Charge Density, and Polarization of Cations on Complex Stability, Solvation Effects And Ion-Pair Formation.

#### **Unit 7: Reactivity and Catalysis**

Reactivity Patterns of Alkali and Alkaline Earth Metal Complexes in Aqueous and Nonaqueous Media, Organometallic Compounds of Alkali and Alkaline Earth Metals: Preparation and Stability. Catalytic Roles in Hydrogenation, Hydroboration, Deprotonation and Enolate Formation, Cross-coupling Reactions (e.g., Kumada and Negishi reactions), Activation of Small Molecules (e.g.,  $H_2$ ,  $CO_2$ , and  $N_2$ ) Using Alkali and Alkaline Earth Metal Complexes.

#### **Unit 8: Biological, Industrial and Environmental Applications**

Complexes of Alkali and Alkaline Earth Metals in Enzymatic Processes and Biomimetic Systems, Industrial applications: Complexes in Ion-exchange Processes, Phase-transfer catalysis, and as



Desiccants, Environmental Applications: Metal Ion Complexes in Water Softening, and Pollutant Sequestration.

### **Block III: Metal pi-Complexes**

#### **Unit 9: Metal Carbonyls**

Metal Carbonyl: Preparation, Properties, Structure and Bonding, Vibrational Spectra of Metal Carbonyls for Bonding and Structural Elucidation, Important Reactions of Metal Carbonyls.

#### **Unit 10: Other Transition Metal**

Preparation, Bonding Structure and Important Reactions of Transition Metal Nitrosyl, Dinitrogen and Dioxygen Complexes; Tertiary Phosphine as Ligand.

#### **Unit 11: Metal-Alkene and Metal-Alkyne Complexes**

Preparation, Properties, Structure and Bonding of Metal-Alkene Complexes, Preparation, Properties, Structure and Bonding of Metal-Alkyne Complexes, Important Reactions and Applications of Metal-Alkene and Metal-Alkyne Complexes in Catalysis and Organic Synthesis, The Dewar-Chatt-Duncanson Model for Metal-Alkene Bonding, Analysis of Vibrational Spectra for Structural Elucidation of Metal-Alkene and Metal-Alkyne Complexes.

#### **Unit 12: Metallocenes and Sandwich Complexes**

Preparation, Properties, Structure, And Bonding of Ferrocene and other Metallocenes, Structure and Bonding of Sandwich Complexes, Including Examples like Dibenzene Chromium and Dibenzene Titanium, Reactivity and Applications of Metallocenes in organic Synthesis and Industrial Catalysis, Concepts of Aromaticity in Metallocenes and their Electronic Structures, Spectroscopic Methods (NMR, IR, UV-Vis) for the Characterization of Metallocenes and Sandwich Complexes.

### **Block IV: Metal Clusters**

#### **Unit 13: Introduction to Metal Clusters**

Definition and Classification of Metal Clusters, Structure of Clusters, Electron Counting In Clusters, Distinction between Low-Valency Metal Clusters (e.g., Metal Carbonyl Clusters) and High-Valency Metal Clusters (E.G., Metal Halide Clusters).

#### **Unit 14: Preparation and Reactions of Metal Clusters**

General Methods for Preparation of Metal Cluster Complexes: Pyrolysis, Electrolytic Reduction, Nucleophilic Attack On Clusters, Reductive Elimination Processes, Reactions Of Metal Clusters: With Electrophiles and Nucleophiles, Oxidative Addition and Reactions on M-M Multiple Bond.

#### **Unit 15: Structure and Bonding**

Structural Aspects of Various Metal Clusters, Metal-Metal Bonding; Including Single, Double, Triple, and Quadruple Bonds, Application of Wade's Rules for Predicting Structures in Higher Boranes and Carboranes.

#### **Unit 16: Boranes and their Derivatives**

Synthesis, Properties, Structure, Bonding, Uses of Higher Boranes, Carboranes, Metalloboranes and Metallocarboranes, Compounds with Metal-Metal Multiple Bonds.

### **Books Recommended/Suggested Readings**

1. J. D. Lee, "Concise Inorganic Chemistry", 5<sup>th</sup> ed., 2008, Oxford University Press, London, UK. ISBN 978-8126515547
2. F.A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, "Advanced Inorganic Chemistry", 6<sup>th</sup> ed., 2007, John Wiley & Sons, Inc. USA. ISBN 978-8126513383
3. R.C. Mehrotra, A. Singh, "Organometallic Chemistry: A Unified Approach", 2<sup>nd</sup> revised ed., 2020, New Age International Publishers. ISBN 978-8122412581

4. B. Douglas, D. McDaniel, J. Alexander, "Concepts and Models of Inorganic Chemistry," 3<sup>rd</sup> ed., 2006, John Wiley & Sons, Inc. USA. ISBN 978-8126509119
5. D. Astruc, "Organometallic Chemistry and Catalysis", 1<sup>st</sup> ed., 2007, Springer USA. ISBN 978-3540461289
6. S. Prakash, G.D. Tuli, S. K. Basu, R. D. Madan, "Advanced Inorganic Chemistry-Volume I", 2021, S Chand & Co. Ltd. ISBN 978-9355010995

### **Course Outcomes**

By the end of this course, students will be able to

1. Apply bonding theories (VBT, CFT, LFT) and VSEPR principles to predict molecular geometries and hybridization in inorganic systems.
2. Analyze the synthesis, structure, and applications of phosphorus-nitrogen, sulfur-nitrogen, and phosphorus-sulfur compounds.
3. Evaluate coordination behavior, stability, and catalytic roles of alkali/alkaline earth metal complexes using HSAB theory and thermodynamic principles.
4. Characterize metal  $\pi$ -complexes (carbonyls, metallocenes) and their bonding models, linking structure to reactivity in organic synthesis and catalysis.
5. Synthesize metal clusters and boranes, correlating their structural features with electron-counting rules and Wade's bonding concepts.
6. Relate inorganic compound design to industrial, environmental, and biological applications, including pollutant sequestration and biomimetic systems.
7. Utilize spectroscopic techniques (IR, NMR, UV-Vis) to probe bonding and structure in metal complexes, clusters, and organometallic systems.

**Course Name: Organic Chemistry- I**

**Code: CHM-6112**

**Credit: 4**

### **Course Objectives**

This course aims to equip students with a comprehensive understanding of stereochemistry, reaction mechanisms, and strategies in organic synthesis. It fosters the ability to analyze molecular symmetry, chirality, and stereoisomerism while developing skills in conformational analysis, asymmetric synthesis, and reaction mechanism determination. By integrating stereochemical principles with synthesis strategies, students will gain proficiency in retrosynthetic analysis, stereoselective synthesis, and the application of these concepts in biological and pharmaceutical sciences.

### **Block I: Stereochemistry I**

#### **Unit 1: Molecular Symmetry and Chirality**

Classification of Stereoisomers; Optical Isomers; Symmetry Operations and Symmetry Elements, Point Group Classification; Symmetry and Molecular Properties; Rotation of Polarised Light, Symmetry Number; Molecules with One Chiral Centre; Chirality and Symmetry

#### **Unit 2: Stereoisomerism of Molecules with More than One Chiral Centres**

Molecules with Two Chiral Centres; Racemic Modifications, Formation (By Mixing, Synthesis, Racemisation etc.), Properties, Different Methods of Resolution, Criteria of Optical Purity; Molecules with Three or More Chiral Centres; Axial and Planar Chirality and Helicity (P and M); Cyclosteroisomerism.

#### **Unit 3: Conformations of Six-membered Rings**

Basic Aspects of Conformations; Stereochemistry of Cycloalkanes; Conformations and Stability of Cyclohexanes; Monosubstituted Cyclohexanes, Disubstituted Cyclohexanes, Trisubstituted Cyclohexanes; Conformations and Stability of Cyclohexenes; Conformations and Stability of Cyclohexanones and Halocyclohexanones; Cyclohexanones, Halocyclohexanones; Conformations and Stability of Decalins, Decalols and Decalones.

#### **Unit 4: Stereochemistry of Complex Systems**

Stereochemistry of Allenes and Spiranes; Stereochemistry of Alkylidines, Stereochemistry of Ethanal, Propanal and Ethyl Methyl Ketone; Stereochemistry of Adamantanes; Stereochemistry of Catenanes; Stereochemistry of Biphenyls, Atropisomerism; Stereochemistry of Bridged Biphenyls; Stereochemistry of Ansa Compounds and Cyclophanes.

### **Block II: Stereochemistry II**

#### **Unit 5: Configuration and its Correlation**

Representation of Configuration: *D*, *L*, *R*, *S* and *E*, *Z* Nomenclature; Determination of Configuration-Different Methods; Chemical Correlation, Quasiracemates.

#### **Unit 6: Topicity and Prostereoisomerism**

Topicity of Ligands and Faces and their Nomenclature; Stereogenicity; Chirogenicity; Pseudoasymmetry; Stereogenic and Prochiral Centres

#### **Unit 7: Asymmetric Induction**

Cram's, Prelog's and Felkin-Ahn Model; Dynamic Stereochemistry (Acyclic and Cyclic); Qualitative Correlation between Conformation and Reactivity; Curtin-Hammett Principle

#### **Unit 8: Molecular Dissymmetry and Chiroptical Properties**

Linear and Circularly Polarised Lights; Circular Birefringence and Circular Dichroism; ORD and CD Curves; Cotton Effect; The Axial Haloketone Rule; Octant Diagrams; Helicity; Lowe's Rule; Application of ORD and CD to Structural and Stereochemical Problems.

### **Block III: Determining Reaction Mechanisms**

#### **Unit 9: Mechanisms of Organic Reactions**

Detailed Mechanisms of Different Organic Reactions, Kinetic and Thermodynamic Control, Hammond's Postulate, Curtin-Hammond Principle, and Reaction Coordinate, Potential Energy Diagrams, Transition States and Intermediates.

**Unit 10: Isotope Effects and Mechanism Determination**

Introduction to Isotope Effects, Theoretical Aspects of Isotope Effects, Experimental Methods to Measure Isotope Effects, Application of Isotope Effects in Mechanism Determination: Case Studies.

**Unit 11: Energy Profiles and Transition State Theory**

Energy Profiles of Chemical Reactions, Transition State Theory and its Applications, Concept of Activation Energy and Arrhenius Equation, Potential Energy Surfaces and Reaction Pathways, Use of Computational Chemistry to Model Transition States and Predict Reaction Outcomes.

**Unit 12: Effect of Structure on Reactivity**

Resonance and Field Effects, Steric Effects and Quantitative Treatments, Hammett Equation and Linear Free Energy Relationships, Substituent and Reaction Constants, Taft Equation.

**Block IV: Strategies of Organic Synthesis**

**Unit 13: Retrosynthesis**

Concept and Significance of Retrosynthetic Analysis, Disconnection Approach, Target Molecule (TM) Identification and Retrosynthetic Tree Construction, Strategic Bond Disconnections: C-C, C-N, C-O and other Key Bonds, Role of Molecular Symmetry, Retrosynthesis of Cyclic and Polycyclic Compounds, Case Studies and Problem-Solving: Retrosynthetic Analysis of Classic and Modern Synthetic Targets (e.g., Taxol, Vancomycin, Artemisinin).

**Unit 14: Control in Synthesis**

Introduction, Protective Groups: Hydroxyl, Amino, Carbonyl, and Carboxylic Acid Protecting Groups, Synthetic Equivalent Groups, Synthetic Analysis and Planning, Control of Stereochemistry, Illustrative Examples.

**Unit 15: Asymmetric Synthesis and Catalysis**

Chiral Auxiliaries, Chiral Pool Synthesis and Chiral Reagents, Overview of Enantioselective Catalysis, Including Organocatalysis, Metal-Catalyzed Asymmetric Synthesis and Biocatalysis, Principles of Enantioselectivity and Diastereoselectivity, Mechanistic Insights into Asymmetric Reactions (e.g., Sharpless Epoxidation, Hydrogenation Using Chiral Ligands and Aldol Reactions, Metrics for Evaluating Enantiomeric Excess and Stereochemical Outcomes.

**Unit 16: Stereochemical Principles in Biological Systems**

Application of Stereochemical Principles in Drug Design and Biological Systems, Stereoselectivity and its Importance in Biological Reactions), Applications of Asymmetric Synthesis in Pharmaceuticals and Materials Science.

**Books Recommended/Suggested Readings**

1. Francis A. Carey and Richard J. Sundberg "Advanced Organic Chemistry; Part A: Structure and Mechanisms", 5<sup>th</sup> ed., 2005, Springer USA. ISBN 978-0387448978
2. Ernest L. Eliel, Samuel H. Wilen, Michael P. Doyle, "Basic Organic Stereochemistry", 2001, 1<sup>st</sup> ed., Wiley-Interscience, USA. ISBN 9780471374992
3. D Nasipuri, "Stereochemistry of Organic Compounds: Principles and Applications", 2012, 4<sup>th</sup> ed., New Academic Science. ISBN 9781906574918
4. P. S. Kalsi, "Stereochemistry: Conformation and Mechanism", 10<sup>th</sup> ed., 2019, New Age International Publishers. ISBN 978-9387788329
5. L.G. Wade Jr., "Organic Chemistry", 2009, 7<sup>th</sup> edition, Pearson Education, USA. ISBN 9780321593919

6. Clayden, J., Greeves, N., & Warren, S., "Organic Chemistry", 2001, 1<sup>st</sup> ed., Oxford University Press, USA. ISBN 9780198503460

### **Course Outcomes**

By the end of this course, students will be able to

1. Analyze molecular symmetry, chirality, and stereoisomerism, applying these principles to complex molecular structures.
2. Evaluate conformational stability in six-membered rings and stereochemical properties of diverse organic systems.
3. Determine molecular configuration using D, L, R, S, and E, Z nomenclature and apply principles of asymmetric induction.
4. Interpret reaction mechanisms through kinetic and thermodynamic analyses, isotope effects, and transition state theory.
5. Utilize retrosynthetic analysis to design synthetic routes for complex organic molecules.
6. Implement stereocontrol strategies in organic synthesis, including the use of protective groups and enantioselective catalysis.
7. Apply stereochemical principles in biological systems, particularly in drug design and materials science.

**Course Objectives**

This course aims to equip students with a fundamental understanding of quantum chemistry, electrochemistry, chemical kinetics, and group theory. It fosters analytical thinking by introducing quantum mechanical principles, model systems, and approximation methods. Students will explore electrochemical cells, electrode kinetics, and ionic interactions, along with reaction dynamics, catalysis, and kinetics in solutions. Additionally, the course provides insights into molecular symmetry, group theory, and their applications in spectroscopy and bonding.

**Block I: Quantum Chemistry****Unit 1: Introduction to Quantum Chemistry**

Historical Background and Need for Quantum Mechanics, Wave-particle Duality, Heisenberg's Uncertainty Principle, Schrodinger's Wave Mechanics: Time-Dependent and Time-Independent Schrödinger Equation, Postulates of Quantum Mechanics; Physical Significance of the Wavefunction, Quantum Mechanical Operators.

**Unit 2: Model Systems**

One-Dimensional Problems: Free Particle, Particle in One and Three Dimensional Box and Harmonic Oscillator.

**Unit 3: Hydrogen like atoms**

Formulation and Solution of the Schrödinger Equation for the Hydrogen Atom, Quantum Numbers and their Significance, Shapes of Orbitals.

**Unit 4: Approximation Methods in Quantum Chemistry**

The Variational Principle, Perturbation Theory, the Hartree-Fock Method, Born-Oppenheimer Approximation, Application of Approximation Methods to Simple Systems (ODB, HO).

**Unit 5: Quantum Mechanics of Multielectron Atoms**

Helium Atom, Ground State Energies, Pauli Exclusion Principle, Antisymmetric Wavefunctions, Many-Electron Atoms, Electronic Configurations, Spin-Orbit Coupling, Slater Determinants.

**Block II: Electrochemistry****Unit 6: Electrochemical Cell-I**

Reversible and Irreversible Cells; EMF and its Experimental Measurement, Electrochemical Cell Representation and Cell Reaction; Types of Electrodes, Nernst Equation and its Importance; Thermodynamics of a Reversible Cell, Calculation of Thermodynamic Properties:  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  from EMF Data; Calculation of Equilibrium Constant from EMF Data.

**Unit 7: Electrochemical Cell-II**

Types of Galvanic Cells and Concentration Cells, Concentration Cells with Transference and Without Transference, Liquid Junction Potential and Salt Bridge, Applications of EMF Measurements Activity Coefficient, Electrolytic Cells.

**Unit 8: Debye Huckel Theory**

Ionic Cloud, Poisson's Equation; Non-Ideality of Electrolytic Solutions, Activity and Mean Activity Coefficient, Measurement of Activity Coefficients; Debye Huckel Theory, Postulates of Debye Huckel Theory, Mathematical Treatment.

**Unit 9: Electrode Kinetics**

Essentials of Electrode Reactions; Butler-Volmer Equation, Derivation of Equation, Significance of Butler-Volmer Equation, Overpotential, Current-Overpotential Equation, Tafel Plot. Electrokinetic phenomena: Electrophoresis and electroosmosis.

### **Block III: Chemical Kinetics**

#### **Unit 10: Collision and Transition State Theories**

Collision theory and Its Limitations, Limitations of Collision Theory, Transition State Theory, Thermodynamic Approach, Statistical Approach.

#### **Unit 11: Theories of Unimolecular Reactions**

Unimolecular Reactions and their Characteristics; Lindemann's Mechanism; Experimental Verification, Limitations of Lindemann's Mechanism; Hinshelwood's Theory, Limitations of Hinshelwood's Theory; RRKM Treatment.

#### **Unit 12: Catalysis and its Applications**

Homogeneous and Heterogeneous Catalysis, Mechanisms of Catalysis: Enzyme Catalysis and Industrial Catalysts, Catalytic Converters and their Applications.

#### **Unit 13: Kinetics of Reactions in Solution**

Solvent Effects on Reaction Rates, Ionic Strength and its Impact on Reaction Kinetics, Diffusion-Controlled Reactions and their Rate Laws.

### **Block IV: Group Theory**

#### **Unit 14: Molecular Symmetry and Groups**

Symmetry Operations and Elements, Molecular Symmetry Elements; Point Groups; Classification of Molecules into Point Groups; Group Multiplication Tables.

#### **Unit 15: Representations of Groups**

Matrix Representation and Its Characteristics; Basis for Representation, Similarity Transformations, Character of Representations, Irreducible Representation, Wavefunction as Basis for Representation Reduced Representation, Reduction of Representation, Symmetry Adapted Basis.

#### **Unit 16: Group Theory in Chemical bonding**

Molecular Orbitals and Symmetry Considerations, Orbital Interactions and Molecular Orbital Diagrams, Application of Group Theory in Transition Metal Complexes.

#### **Unit 17: Applications of Group Theory in Spectroscopy**

Application of Character Tables in Determining Molecular Properties, Vibrational Modes and Selection Rules, Electronic Spectroscopy.

### **Books Recommended/Suggested Readings**

1. Donald A McQuarrie, "Quantum Chemistry", 2<sup>nd</sup> ed., 2008, University Science Books, Sausalito, California. ISBN 978-1-891389-50-4
2. Ira N. Levine, "Quantum Chemistry", 7<sup>th</sup> ed., 2014, Pearson Education Inc., USA. ISBN 978-0-321-80345-0
3. R. K. Prasad, "Quantum Chemistry", 4<sup>th</sup> revised edition, 2020, New Age International Publishers. ISBN 978-8122424089
4. Allen J. Bard, Larry R. Faulkner, "Electrochemical Methods: Fundamentals and Applications", 3<sup>rd</sup> ed., 2022, John Wiley & Sons Ltd. USA. ISBN: 978-0-471-04372-0
5. Peter Atkins, Julio De Paula, "Physical Chemistry", 9<sup>th</sup> ed., 2010, W. H. Freeman and Company, New York, USA. ISBN 978-1-429-21812-2
6. Keith J. Laidler, "Chemical Kinetics", 3<sup>rd</sup> ed., 2003, Pearson Education India. ISBN: 978-8131709726
7. F. Albert Cotton, "Chemical Applications of Group Theory", 3<sup>rd</sup> edition, 1990, John Wiley & Sons Inc., USA. ISBN 0-471-51094-7

### **Course Outcomes**

By the end of this course, students will be able to

1. Apply quantum mechanical principles to model systems, hydrogen-like atoms, and multi-electron atoms.
2. Analyze electrochemical cells, calculate thermodynamic parameters from EMF data, and understand electrode kinetics.
3. Explain and apply the Debye-Hückel theory to ionic interactions in electrolytic solutions.
4. Interpret reaction kinetics using collision theory, transition state theory, and unimolecular reaction mechanisms.
5. Evaluate catalytic processes, including enzyme catalysis and industrial catalytic applications.
6. Utilize group theory to classify molecules, predict molecular properties, and analyze chemical bonding.
7. Apply character tables in spectroscopy to determine vibrational modes and selection rules.



**Course Name: Analytical Chemistry- I**

**Code: CHM-6114**

**Credits: 4**

### **Course Objectives**

This course aims to provide students with a comprehensive understanding of analytical chemistry principles and techniques. It focuses on measurement accuracy, data analysis, quality control, and laboratory safety, alongside classical and modern separation and electroanalytical methods. Through this course, students will develop the ability to apply various techniques, such as titrations, chromatography, and voltammetry, to solve real-world analytical problems, ensuring precision and reproducibility in laboratory results.

### **Block I: Fundamentals of Analytical Chemistry**

#### **Unit 1: Measurement Basics and Data Analysis**

Accuracy, Precision, Sensitivity and Specificity, Types of Errors: Systematic, Random and Gross Errors, Minimization of Errors, Significant Figures and Rounding Off, Gaussian Distribution of Data, Standard Deviation, Relative Standard Deviation, Confidence Intervals, Criteria for Rejection of Data (Q-Test, T-Test, F-Test and Chi-Square Test), Control Charts and Statistical Treatment of Data.

#### **Unit 2: Sampling and Standard Reference Materials**

Sampling Methods: Random, Stratified and Systematic Sampling, Sampling Errors and their Minimization, Preparation and Use of Standard Reference Materials (SRMs), Role of SRMs in Quality Control and Validation.

#### **Unit 3: Laboratory Techniques and Safety**

Basic Laboratory Equipment: Balance, pH Meter, Volumetric Apparatus and Spectrophotometers; Good Laboratory Practices (GLP): Laboratory Organization, Sample Handling and Record-Keeping; Safety Protocols: Chemical Hazards, Personal Protective Equipment (PPE) and Waste Disposal.

#### **Unit 4: Quality Assurance and Quality Control**

Ensuring Accuracy and Reproducibility in Analytical Results, Standard Operating Procedures (SOPs): Importance in Achieving Reliable Results, Internal and External Quality Control: Use of Control Samples, Proficiency Testing and Certification, Good Manufacturing Practices (GMP): Regulatory Frameworks and their Importance in Analytical Laboratories.

### **Block II: Classical Analytical Methods**

#### **Unit 5: Acid-Base Equilibria**

Monoprotic and Polyprotic Systems, Neutralization Reactions, Buffer Solutions and their Preparation, Buffer Capacity, Theory of Acid-Base Indicators, Acid-Base Titrations, Some Applications of AB Titrations.

#### **Unit 6: Redox Equilibrium**

Redox Reaction and Redox Potential; Redox Equilibrium Constant; Redox Titration Curves; Redox Indicators, Some Applications of Redox Titrations.

#### **Unit 7: Complexometric Titrations**

Metal Complex Equilibria; Formation Constants and Stability of Complexes; EDTA Equilibria, Metallochromic Indicators, Types of EDTA Titrations, Some Applications of Complexometric Titrations.

#### **Unit 8: Precipitation Titrations**

Mohr's and Volhard's methods, Precipitation from Homogeneous Solutions, Organic Precipitants: Advantages and Disadvantages, Some Applications of Precipitation Titrations.

### **Block III: Separation Techniques-I**

**Unit 9: Liquid-Liquid Extraction**

Nernst Distribution Law and Distribution Coefficient, Separation Factor and Factors Affecting Extraction, Extraction Systems for Metal Ion Separations, Batch, Continuous and Counter-Current Extraction, Limitations of Liquid-Liquid Extraction.

**Unit 10: Solid Phase Extraction**

Basic SPE Procedure: Loading, Washing and Elution, Optimization of Extraction Conditions (pH, Solvent Polarity, Flow Rate, Sample Volume, Sorbent Selection Etc.), Types of Extraction: Off-Line, On-Line and Automated SPE, Common Solvents Used in the Elution, Types of SPE, Applications of SPE, Advantages and Limitations of SPE.

**Unit 11: Thin layer chromatography (TLC)**

Thin Layer Chromatography (TLC) - Fundamentals and Principles of Thin Layer Chromatography (TLC), Mobile- Stationary Phases, Normal- Reverse Phases, Visualizing Reagent (KMnO<sub>4</sub>, Ninhydrin, DD and Others), Applicability and Importance with Examples.

**Unit 12: Size Exclusion Chromatography (SEC)**

Introduction to SEC, Fundamentals of Separation Mechanism, Stationary Phase Materials: Types and Properties, Mobile Phase Considerations, Instrumentation, Applications of SEC, Advantages and Limitations of SEC, Recent Advances and Developments.

**Block IV: Separation and Electroanalytical Techniques****Unit 13: Gas Chromatography (GC)**

Gas Chromatography (GC) - Fundamentals and Principles of Gas Chromatography (GC), Instrumentation, Sample Preparation, Carrier Gases, Injectors (Split/Splitless, PTV, Head Space, Pyrolyzer and others), Pack and Capillary Columns, Detectors (TCD, FID, ECD, NPD, TEA, Ion Mobility Scan), Applications and Importance with Examples, Limitations.

**Unit 14: High Performance Liquid Chromatography (HPLC)**

High Performance Liquid Chromatography (HPLC): Fundamentals and Principles of High Performance Liquid Chromatography (HPLC), Instrumentation, Types of HPLC—Normal Phase HPLC, Reverse Phase HPLC, Mobile Phases, Sample Preparation, Limitations of HPLC, HPLC Injectors, HPLC Pumps, HPLC Columns, HPLC Detectors (UV-Visible, Fluorescence, PDA, RI and others).

**Unit 15: Polarography**

Polarography- Principles, Ilkovic Equation, Factors Affecting on Polarographic Wave, Application.

**Unit 16: Voltammetry**

Voltammetry - Principle, Cyclic Voltammetry, Criteria of Reversibility of Electrochemical Reactions, Quasi-Reversible and Irreversible Processes, Application

**Unit 17: Coulometry**

Coulometry: Principles, Types of Coulometric Methods; Controlled Potential Coulometry, Constant Current Coulometry; Applications of Coulometric Methods.

**Books Recommended/Suggested Readings**

1. Gary D Christian, Purnendu Dasgupta, Kevin Schug, "Analytical Chemistry", 7<sup>th</sup> ed., 2014, John Wiley & Sons, Inc. USA. ISBN 978-0-470-88757-8
2. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, "Fundamentals of Analytical Chemistry", 9<sup>th</sup> ed., 2014, Brooks/Cole Belmont CA USA. ISBN 978-0-495- 55828-6
3. David Harvey, "Modern Analytical Chemistry", 2000, The McGraw-Hill Companies Inc. ISBN 0-07-237547-7
4. Allen J. Bard, Larry R. Faulkner, "Electrochemical Methods: Fundamentals and Applications", 3<sup>rd</sup> ed., 2022, John Wiley & Sons Ltd. USA. ISBN: 978-0-471-04372-0

5. Daniel. C. Harris, "Quantitative Chemical Analysis" 9<sup>th</sup> ed., 2015, W. H. Freeman & Co Ltd. ISBN 978-1464135385
6. J. Mendham, R. C. Denny, M. Thomas, B. Sivasankar, "Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> ed., 2009, Pearson Education Ltd. ISBN 978-8131723258
7. H. M. McNair, James M. Miller, " Basic Gas Chromatography", 2<sup>nd</sup> ed., 2009, Wiley-Blackwell Ltd. ISBN 978-0470439548
8. R. Kalvoda, "Electroanalytical Methods in Chemical and Environmental Analysis", 1987, Kluwer Academic/Plenum Publishers. ISBN 978-0306417993

### **Course Outcomes**

By the end of this course, students will be able to

1. Understand and apply the principles of accuracy, precision, and error minimization in analytical measurements.
2. Demonstrate knowledge of various sampling methods and the role of Standard Reference Materials in quality control.
3. Gain practical skills in laboratory techniques, including the use of balances, pH meters, and spectrophotometers.
4. Develop the ability to apply quality assurance protocols, including SOPs, GMP, and proficiency testing.
5. Master classical analytical methods like acid-base, redox, complexometric, and precipitation titrations.
6. Implement advanced separation techniques such as liquid-liquid extraction, solid-phase extraction, and chromatography.
7. Understand and apply electroanalytical techniques, including polarography, voltammetry, and coulometry, to analyze chemical systems.

**Course Objectives**

This course aims to provide students with hands-on experience in the preparation and analysis of organic compounds, along with the practical application of various analytical techniques. Through the synthesis of compounds via reactions such as the Cannizzaro reaction, oxidation, aldol condensation, acetylation, and diazotization, students will gain insights into reaction mechanisms and product characterization. Additionally, the course includes the estimation of water hardness and chromatographic separation of amino acids, equipping students with essential analytical skills.

**Organic Chemistry****Preparation- (any four of the following)**

1. Cannizzaro Reaction: 4-Chlorobenzaldehyde as Substrate.
2. Oxidation: Adipic Acid By Chromic Acid Oxidation of Cyclohexanol
3. Aldol Condensation: Dibenzalacetone / Chalcone from Benzaldehyde
4. Acetylation: Acetylation of Cholesterol
5. Diazotisation Reaction of Naphthylamine
6. Friedel Crafts Reaction: -Benzoylpropionic Acid from Succinic Anhydride and Benzene.
7. Sandmeyer Reaction: Starting from Naphthylamine
8. Acetoacetic Ester Condensation of Ethyl Acetate with Benzaldehyde

**Analytical Chemistry**

1. Estimation of Total, Temporary and Permanent Hardness of the Given Water Sample by EDTA Method.
2. Paper Chromatographic Separation and Identification of Amino Acids from their Mixture.

**Books Recommended/Suggested Readings**

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry" 5<sup>th</sup> ed., 2003, Pearson India Ltd. ISBN 9788177589573
2. J. Leonard, B. Lygo, G. Procter "Advanced Practical Organic Chemistry" 3<sup>rd</sup> ed., 2013, CRC Press. ISBN 978-1439860977
3. Daniel. C. Harris, "Quantitative Chemical Analysis" 9<sup>th</sup> ed., 2015, W. H. Freeman & Co Ltd. ISBN 978-1464135385

**Course Outcomes**

1. Students will be able to independently perform various organic synthesis reactions, understand their mechanisms, and characterize the products.
2. Students will acquire skills in analytical techniques such as EDTA titration for water hardness estimation and paper chromatography for amino acid separation.
3. Students will develop critical thinking and problem-solving abilities by troubleshooting experimental procedures and interpreting analytical data effectively.

**Course Objectives**

The primary objective of this laboratory course is to equip M.Sc. Chemistry students with the practical skills necessary to detect, separate, and quantify less common and common metal ions using various analytical techniques. Additionally, students will gain hands-on experience in potentiometric, pH-metric, and conductometric titrations to determine the properties and behaviors of different chemical species. This comprehensive training will enhance students' analytical capabilities and understanding of inorganic and physical chemistry principles through experimental practice.

**Inorganic Chemistry**

1. Detection of Less Common Metal Ions: Ce, Ti, Mo, W, Zr, Th, V, U, (Two Metal Ions in Cationic/Anionic Forms: Minimum Two Mixtures).
2. Separation and Determination of Two Metal Ions (Ca, Mg, Cu, Ni, Zn, Cu, Pb) Involving Volumetric Titrations (Redox & Complexometry) and Gravimetry (Minimum Three Experiments).

**Physical Chemistry**

1. Titrate Potentiometrically a Solution of Ferrous Ions (Mohr's Salt) Against  $\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ .
2. Determine The Dissociation Constant ( $pK_a$ ) of a Weak Acid Using a *pH* Meter
3. Study The Conductometric Titration of:
  - i. Hydrochloric Acid vs. Sodium Hydroxide
  - ii. Acetic Acid vs. Sodium Hydroxide,
  - iii. Acetic Acid vs. Ammonium Hydroxide,
4. Study the Stepwise Neutralization of a Polybasic Acid e.g. Oxalic Acid, Citric Acid, Succinic Acid (Any One) By Conductometric Titration and Explain the Variation in the Plots.

**Books Recommended/Suggested Readings**

1. J. Mendham, R. C. Denny, M. Thomas, B. Sivasankar, "Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> ed., 2009, Pearson Education Ltd. ISBN 978-8131723258
2. Daniel. C. Harris, "Quantitative Chemical Analysis" 9<sup>th</sup> ed., 2015, W. H. Freeman & Co Ltd. ISBN 978-1464135385
3. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, "Fundamentals of Analytical Chemistry", 9th edition, 2014, Brooks/Cole Belmont CA USA. ISBN 978-0-495-55828-6

**Course Outcomes**

1. Students will develop proficiency in the detection and separation of metal ions, utilizing volumetric, gravimetric, and instrumental analysis methods to achieve accurate and reliable results.
2. By conducting various titrations and determining chemical properties such as dissociation constants and neutralization behaviors, students will enhance their ability to solve complex chemical problems through analytical reasoning and data interpretation.
3. The hands-on laboratory experience will bridge the gap between theoretical concepts and real-world applications, preparing students for advanced research and professional practice in the field of chemistry.

## SEMESTER: II

Course Name: Inorganic Chemistry – II

Code: CHM-6211

Credit: 4

### Course Objectives

This course aims to provide a comprehensive understanding of metal-ligand bonding, electronic spectroscopy, magnetism, and reaction mechanisms in coordination chemistry, while connecting theory to real-world applications. Students will master foundational concepts like Crystal Field and Molecular Orbital theories, interpret electronic spectra and magnetic behavior, and analyze substitution mechanisms in diverse geometries. The course also explores bioinorganic chemistry, emphasizing the role of metalloproteins, enzymes, and metal-based drugs in biological systems. By integrating theory, spectroscopy, and practical case studies, students will develop the skills to predict stability, reactivity, and functional properties of metal complexes, preparing them for advanced research or industrial applications.

### Block I: Metal-Ligand Bonding

#### Unit 1: Theories of Metal-Ligand Bonding

Crystal Field Theory and its Limitations, Molecular Orbital Theory, Octahedral, Tetrahedral and Square Planar Complexes, Jahn-Teller Effect, pi-Bonding and Molecular Orbital Theory, Spectrochemical Series, Low Spin and High Spin Complexes.

#### Unit 2: Crystal Field Stabilization and Related Aspects

Crystal Field Stabilization Energy, Spectrochemical Series, Weak and Strong Field Complexes, Thermodynamic and Related Aspects of Crystal Fields, Ionic Radii, Heats of Ligation, Lattice Energies, Site Preference Energies.

#### Unit 3: Stability of Metal Complexes

Factors Affecting the Stability of Metal-Ligand Complexes Including Charge Density, Ligand Size, and Electronegativity, Chelate Effect and Thermodynamic Origins.

### Block II: Electronic Spectroscopy and Magnetism

#### Unit 4: Electronic Spectroscopy of Transition Metal Complexes

Fundamentals of Electronic Spectra, Absorption of Light and Electronic Transitions, Types of Electronic Transitions: d-d, Charge Transfer (MLCT and LMCT) and Others, Crystal Field Theory and Spectra, Term Symbols and Multiplicity, Selection Rules.

#### Unit 5: Interpretation of Electronic Spectra

Spectroscopic Ground States, Correlation, Orgel and Tanabe-Sugano Diagrams for Transition Metal Complexes ( $d^1$ - $d^9$  States), Calculations of Racah Parameters.

#### Unit 6: Applications of Electronic Spectroscopy

Spectroscopic Method of Assignment of Absolute Configuration in Optically Active Metal Chelates and their Stereochemical Information, Electronic Spectra of Metalloproteins and Enzymes, Time-Resolved Spectroscopy, Analysis of Complex Spectra, Comparative Study of High Spin vs. Low Spin Systems.

#### Unit 7: Fundamentals of Magnetism in Transition Metals

Definition and Types of Magnetism: Diamagnetism, Paramagnetism, Ferromagnetism, Antiferromagnetism and Ferrimagnetism, Origin of Magnetic Moments, Determination of Magnetic Moments Using the Gouy Balance Method and the Faraday Method, Concept of Magnetic Susceptibility, Application of the Curie and Curie-Weiss Laws.

#### Unit 8: Magnetic Behavior of Transition Metal Complexes

Magnetic Properties of Complexes of Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn, Spin Crossover and Jahn-Teller Effect, Introduction to Molecular Magnets, Single-Molecule Magnets (SMMs) and Single-Chain Magnets (SCMs).

### **Block III: Reaction Mechanisms of Metal Complexes**

#### **Unit 9: Substitutions in Square Planar Complexes**

Mechanisms of Substitution Reactions of Square Planar complexes: Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects, Berry's Pseudo Rotation Mechanism; Factors Affecting the Reactivity of Square Planar Complexes, Swain-Scott Equation.

#### **Unit 10: Substitutions in Square Pyramidal and Trigonal Bipyramidal Complexes**

Mechanisms of Substitution Reactions of Square Pyramidal and Trigonal Bipyramidal Complexes: Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects.

#### **Unit 11: Substitutions in Octahedral and Tetrahedral Metal Complexes**

Mechanisms of Substitution Reactions of Octahedral Complexes: Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects, Trans Effect and its Application to Synthesis of Complexes; Stereochemical Changes in Substitution Reactions of Octahedral and Tetrahedral Complexes.

#### **Unit 12: Molecular Rearrangements**

Molecular Rearrangement Processes; Electron Transfer Reactions (Outer and Inner Sphere); HOMO and LUMO of Oxidant and Reductant, Chemical Activation, Precursor Complex Formation and Rearrangement; Nature of Bridged Ligands; Fission of Successor Complexes, Two-Electron Transfers.

### **Block IV: Bioinorganic Chemistry**

#### **Unit 13: Fundamentals of Bioinorganic Chemistry**

Historical Development and Significance, Role of Metal Ions in Biological Systems, Metal Ion Transport and Storage, Metal Ion Interactions with Nucleic Acids.

#### **Unit 14: Metalloproteins and Their Functions**

Hemoglobin and Myoglobin, Iron-Sulfur Proteins, Copper Proteins, Zinc Proteins.

#### **Unit 15: Metalloenzymes and Catalysis**

Mechanisms of Metalloenzymes, Role of Metal Ions in Enzyme Catalysis, Structure and Function of Key Metalloenzymes, Biomimetic Models and their Applications.

#### **Unit 16: Medicinal Aspects of Bioinorganic Chemistry**

Metal-Based Drugs and their Mechanisms of Action, Diagnostic Applications of Metal Complexes (e.g. MRI Contrast Agents), Advanced Spectroscopic Techniques in Bioinorganic Chemistry: X-Ray Crystallography, NMR, EPR and Mössbauer Spectroscopy for Studying Metalloprotein Structures and Functions.

### **Books Recommended/Suggested Readings**

1. F.A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, "Advanced Inorganic Chemistry", 6<sup>th</sup> ed., 2007, John Wiley & Sons, Inc. USA. ISBN 978-8126513383
2. G. L. Miessler, P. J. Fischer, D. A. Tarr "Inorganic Chemistry" 3<sup>rd</sup> ed., 2008, Pearson India Ltd. ISBN 978-8131718858
3. J. E. Huheey, E. A. Keiter, R. A. Keiter, O. K. Medhi, "Inorganic Chemistry: Principles of Structure and Reactivity", 5<sup>th</sup> ed., 2022, Pearson Education Ltd., ISBN 13 978-9356064485
4. R. B. Jordan, "Reaction Mechanisms of Inorganic and Organometallic Systems", 2<sup>nd</sup> ed., 1998, Oxford University Press, USA. ISBN 978-0195115550
5. D. Rehder, "Bioinorganic Chemistry", 2014, Oxford University Press. ISBN 978-0199655199

### **Course Outcomes**

Upon successful completion of this course, students will be able to

1. Explain the principles of Crystal Field and Molecular Orbital theories to predict geometries, stability, and electronic transitions in metal complexes.
2. Interpret electronic spectra using Orgel/Tanabe-Sugano diagrams and correlate spectral data with metal oxidation states, ligand effects, and spin states.
3. Analyze magnetic properties of transition metal complexes using susceptibility measurements and relate them to electronic configurations and ligand-field effects.
4. Evaluate substitution reaction mechanisms (square planar, octahedral, etc.) by interpreting potential energy diagrams, isotope effects, and stereochemical changes.
5. Assess the biological roles of metalloproteins and metalloenzymes, including their structural, catalytic, and medicinal applications.
6. Apply spectroscopic techniques (EPR, NMR, X-ray) and thermodynamic principles to determine stability, reactivity, and functional behavior of coordination compounds.



**Course Name: Reactions and Mechanisms in Organic Chemistry****Code: CHM-6212****Credits: 4****Course Objectives**

This course aims to provide a comprehensive understanding of the mechanistic aspects of organic reactions, including nucleophilic and electrophilic substitution, elimination, addition, free radical, and pericyclic reactions. Students will gain in-depth knowledge of reaction mechanisms, factors affecting reactivity, stereochemical outcomes, and the synthetic applications of various organic reactions. The course is designed to equip students with the skills to analyze and predict reaction pathways and develop a strong foundation in advanced organic chemistry.

**Block I: Nucleophilic Substitution Reactions****Unit 1: Aliphatic Nucleophilic Substitution Reactions**

$S_N2$  Reactions,  $S_N1$  Reactions,  $S_Ni$  Reactions, Factors Affecting  $S_N1$ ,  $S_N2$  and  $S_Ni$  Reactions, Stereochemical Outcomes, Comparative Study of  $S_N1$  and  $S_N2$  Mechanism, SET (Single Electron Transfer) Mechanism.

**Unit 2: Neighboring Group Participation and Carbocation Rearrangements**

Concept and Examples of Neighbouring Group Participation (NGP) in Aliphatic Substitution, Evidence for NGP: Kinetic and Stereochemical Studies, Mechanistic Aspects of NGP, Common Reactions involving NGP: Hydrolysis of Esters and Lactones, Reactions of Halides with Neighboring Groups, Mechanisms of Rearrangements : Hydride shift, alkyl shift, ring expansion and contractions, Experimental Evidence for Carbocation Rearrangements, Applications of Carbocation Rearrangements in Organic Synthesis.

**Unit 3: Nucleophilic Substitution at Unsaturated and Strained Systems**

Substitutions at Allylic, Aliphatic Trigonal, and Vinylic Carbons, Factors Affecting Reactivity, Mechanistic Pathways and Challenges, Substitution in Strained Systems (e.g., Cyclopropyl and Cyclobutyl Carbons).

**Unit 4: Aromatic Nucleophilic Substitution Reactions**

$S_NAr$  (Aromatic Nucleophilic Substitution via Addition-Elimination),  $S_Ni$  (Aromatic Nucleophilic Substitution via Substitution-Nucleophilic Internal), Benzyne Mechanism,  $S_NR_i$  (Aromatic Nucleophilic Substitution via Radical Intermediate), Reactivity Effects, Special Rearrangements (Von Richter, Sommelet-Hauser, Smiles, Meisenheimer and Bamberger).

**Block II: Electrophilic Substitution Reactions****Unit 5: Aliphatic Electrophilic Substitution Mechanisms**

Bimolecular Mechanisms:  $S_E2$  and  $S_{Ei}$ ,  $S_{E1}$  Mechanism, Electrophilic Substitution Accompanied by Double Bond Shifts, Addition-Elimination Mechanism, Factors Affecting Reactivity: Substrates, Leaving Groups, and Solvent Polarity.

**Unit 6: Aromatic Electrophilic Substitution Mechanisms**

The Arenium Ion Mechanism, Orientation and Reactivity in Electrophilic Aromatic Substitution, Energy Profile Diagrams for Aromatic Electrophilic Substitution, The Ortho/Para Ratio, Ipso Attack, Orientation in Other Ring Systems (e.g. Heteroaromatics).

**Unit 7: Quantitative Treatment of Reactivity**

Quantitative Analysis of Reactivity in Substrates and Electrophiles, Use of Hammett Equation and Other Linear Free Energy Relationships in Aromatic Substitution, Application of Substituent Constants and Reaction Constants, Factors Influencing Electrophilic Aromatic Substitution Rates and Selectivity.

**Unit 8: Name Reactions**

Diazonium Coupling Reactions, Vilsmeier-Haack Reaction, Gattermann-Koch Reaction, Other Named Electrophilic Substitution Reactions (e.g., Friedel-Crafts Acylation, Alkylation, Kolbe-Schmitt, And Hell-Volhard-Zelinsky), Reaction Pathways and Synthetic Applications of these Reactions.

### **Block III: Elimination and Addition Reactions**

#### **Unit 9: Elimination Reactions**

The E2, E1, E1cB, and E2C Reactions, Orientation of the Double Bond, Reactivity Effects of Substrate Structures, Attacking Base, The Leaving Group, and the Medium, Mechanism and Orientation in Pyrolytic Elimination: Saytzeff, Hoffman, and Cope elimination.

#### **Unit 10: Addition to Carbon-Carbon Multiple Bonds**

Mechanistic and Stereochemical Aspects of Addition Reactions Involving Electrophiles, Nucleophiles, and Free Radicals, Regio and Chemoselectivity, Orientation and Reactivity, Addition to the Cyclopropane Ring, Hydrogenation of Double and Triple Bonds, Hydrogenation of Aromatic Rings, Hydroboration and Related Reactions, Michael Addition and Sharpless Asymmetric Epoxidation.

#### **Unit 11: Addition to Multiple Bonds with Hetero Atoms**

Mechanism of Metal Hydride Reduction of Saturated and Unsaturated Carbonyl Compounds, Acid Esters and Nitriles, Addition of Grignard Reagents, Reformatsky Reaction and Related Reactions, Mechanism of Wittig Reaction, Knoevenagel, Claisen, Mannich, Stobbe Reactions, Stork Enamine Reaction, Concept and Applications of Umpolung and Sulfur Ylides.

#### **Unit 12: Stereochemical Aspects of Elimination and Addition Reactions**

Stereochemistry of Elimination and Addition Reactions, Influence of Neighboring Groups and Steric Effects on Reaction Pathways, Comparative Analysis of Elimination versus Substitution Reactions, Pericyclic Elimination Reactions and their Stereochemical Outcomes.

### **Block IV: Free Radical and Pericyclic Reactions**

#### **Unit 13: Free Radical Reactions**

Types of Free Radical Reactions, Mechanism of Free Radical Substitution, Reactions on Aromatic Substrates, Neighboring Group Assistance, Reactivity for Aliphatic and Aromatic Substrates at a Bridgehead Carbon, Reactivity of the Attacking Radicals and the Effect of Solvents on Reactivity.

#### **Unit 14: Specific Free Radical Reactions**

Allylic Halogenation (NBS), Oxidation of Aldehydes to Carboxylic Acids, Auto-Oxidation, Coupling of Alkynes and Arylation of Aromatic Compounds by Diazonium Salts, Sandmeyer Reaction, Free Radical Rearrangement and The Hunsdiecker Reaction.

#### **Unit 15: Fundamentals of Pericyclic Reactions**

Definition and Classification (Cycloaddition, Electrocyclic, Sigmatropic, and Group Transfer Reactions), Concerted Mechanisms and Transition State Concepts, Molecular Orbital Interactions in Pericyclic Reactions, Selection Rules for Pericyclic Reactions (Thermal versus Photochemical Conditions), Supra-Supra and Antarafacial Interactions, Hückel and Möbius Aromaticity in Transition States.

#### **Unit 16: Pericyclic Reactions and their Applications**

Diels-Alder Reaction, [2+2] and [4+4] Cycloaddition Reactions, Ring-Closing and Ring-Opening Reactions, [1,3], [1,5], [3,3]-Sigmatropic Shifts, Cope and Claisen Rearrangements, Group Transfer and Chelotropic Reactions, Reaction Pathways and Applications of these Reactions in Organic Synthesis.

### **Books Recommended/Suggested Readings**

1. Francis A. Carey and Richard J. Sundberg "Advanced Organic Chemistry; Part A: Structure and Mechanisms", 5<sup>th</sup> ed., 2005, Springer USA. ISBN 978-0387448978
2. L.G. Wade Jr., "Organic Chemistry", 2009, 7th edition, Pearson Education, USA. ISBN 9780321593919
3. Clayden, J., Greeves, N., & Warren, S., "Organic Chemistry", 2001, 1<sup>st</sup> ed., Oxford University Press, USA. ISBN 9780198503460
4. M. B. Smith, "March's Advanced Organic Chemistry: Reactions Mechanisms and Structure", 7<sup>th</sup> ed., 2015, John Wiley & Sons Inc. USA. ISBN 978-8126556588
5. I. Fleming, "Pericyclic Reactions" 2<sup>nd</sup> ed., 2015, Oxford University Press. ISBN 978-0199680900

### **Course Outcomes**

1. Students will be able to understand and analyze the mechanisms of various organic reactions, including nucleophilic and electrophilic substitutions, eliminations, additions, free radical reactions, and pericyclic reactions.
2. Students will develop the ability to predict reaction pathways and outcomes based on mechanistic understanding and stereochemical considerations, enabling them to design and optimize organic syntheses.
3. Students will be able to apply theoretical concepts such as the Hammett equation, linear free energy relationships, and molecular orbital interactions to explain and predict the reactivity and selectivity of organic reactions.
4. Through the study of specific reactions and problem-solving exercises, students will acquire the skills to synthesize complex organic molecules, utilizing a variety of reactions and mechanistic insights to achieve desired transformations efficiently.

**Course Objectives**

This course aims to build a robust foundation in thermodynamics and statistical mechanics, equipping students to analyze energy transformations, equilibrium, and entropy in chemical and biological systems. Students will explore core concepts like Gibbs energy, chemical potential, partition functions, and irreversible processes, while connecting statistical mechanics to macroscopic properties of gases and solids. Emphasis is placed on applying principles to real-world phenomena, including photochemical reactions, transport processes, and biological energy dynamics. By integrating theory with problem-solving, the course fosters critical thinking skills to evaluate thermodynamic stability, predict reaction behavior, and quantify energy dissipation in complex systems.

**Block I: Thermodynamics and Statistical Thermodynamics****Unit 1: Fundamentals of Thermodynamics and Energy Functions**

Review of Thermodynamics, Internal Energy, Enthalpy and Entropy; Laws of Thermodynamics Gibbs and Helmholtz's Functions; Gibb's Function and Equilibrium Criterion; Temperature and Pressure Dependence of Gibb's Energy; Helmholtz Function and Equilibrium Criterion

**Unit 2: Chemical Potential and Systems of Variable Composition**

Systems of Variable Composition: Partial Molar Quantities and their Significance, Experimental Determination Partial Molar Volume; Chemical Potential, Significance of Chemical Potential; Mixture of Gases, Concept, and Determination of Fugacity; Gibbs-Duhem Equation.

**Unit 3: Heat Capacities and the Third Law of Thermodynamics**

Specific Heat of Solids: Einstein and Debye Models of Heat Capacities of Monatomic Solids, Temperature Dependence of Heat Capacities in Solids, Third Law of Thermodynamics: Residual Entropy and its Significance, Applications of the Third Law in Determining the Absolute Entropy of Substances.

**Unit 4: Fundamentals of Statistical Mechanics**

Role and Importance of Statistical Mechanics in Chemistry, Basic Concepts of Statistical Mechanics: Microstates and Macrostates, Thermodynamic Probability and the Concept of Distribution, Types of Statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Statistics, Thermodynamic Probability ( $W$ ) for the three Types of Statistics.

**Block II: Applied Statistical Mechanics and Thermodynamics****Unit 5: Distribution Laws and Molecular Partition Functions**

Derivation of Distribution Laws (Most Probable Distribution) For Maxwell-Boltzmann, Bose-Einstein, And Fermi-Dirac Statistics, Lagrange's Undetermined Multipliers And Stirling's Approximation, Concept And Calculation Of The Molecular Partition Function, Importance Of The Partition Function In Determining Thermodynamic Properties.

**Unit 6: Applications of Statistical Mechanics to Ideal Gases**

The Molecular Partition Function and its Factorization, Evaluation of Translational, Rotational and Vibrational Partition Functions For Monatomic, Diatomic and Polyatomic Gases, Electronic and Nuclear Partition Functions, Calculation of Thermodynamic Properties of Ideal Gases in Terms of The Partition Function (Internal Energy, Entropy, Helmholtz Free Energy), Statistical Definition of Entropy and its Calculation for Ideal Gases.

**Unit 7: Equilibrium and Thermodynamic Properties**

Calculation of equilibrium constants of gaseous solutions in terms of the partition function, Perfect gas mixtures and their thermodynamic properties, Relationship between the partition function and the

thermodynamic potentials (Gibbs free energy, enthalpy), Statistical approach to chemical equilibrium and reaction rates.

#### **Unit 8: Advanced Topics in Statistical Thermodynamics**

Phase Space and the Concept of Ensembles: Microcanonical, Canonical and Grand Canonical Ensembles, Relationship between Partition Functions and Thermodynamic Functions, Fluctuations and their Significance in Statistical Mechanics, Basics of the Ising Model and Lattice Statistics, Introduction to Non-Equilibrium Statistical Mechanics and Transport Properties.

### **Block III: Irreversible Thermodynamics**

#### **Unit 9: Introduction to Irreversible Thermodynamics**

Meaning and Scope of Irreversible Thermodynamics, Thermodynamic Criteria for Non-Equilibrium States, Concept of Entropy Production and Entropy Flow, Entropy Balance Equation for Different Irreversible Processes (e.g., Heat Flow, Chemical Reaction, Flow of Electricity), Relationship between Equilibrium and Non-Equilibrium Thermodynamics.

#### **Unit 10: Phenomenological Laws and Linear Thermodynamics**

Phenomenological Laws of Irreversible Processes, Linear Laws: Onsager's Relations, Fluxes and Forces in Thermodynamic Systems, Derivation and Application of the Generalized Flux-Force Equations for Uncoupled and Coupled Processes, Gibbs Equation for Non-Equilibrium Thermodynamic Systems, Transformation of Generalized Fluxes and Forces in Irreversible Processes.

#### **Unit 11: Microscopic Reversibility and Non-equilibrium Stationary States**

Principle of Microscopic Reversibility and Onsager's Reciprocity Relations, Non-Equilibrium Stationary States and their Characteristics, Stability of Non-Equilibrium States and Criteria for their Existence, Applications of Onsager's Relations in Thermodynamic Systems, Prigogine's Principle of Maximum Entropy Production and its Implications.

#### **Unit 12: Irreversible Thermodynamics in Biological Systems**

Application of Irreversible Thermodynamics to Biological Systems, Electrokinetic Phenomena and their Relevance to Biological Processes, Energy Dissipation in Biological Systems: Transport Phenomena in Living Organisms, Case Studies: Osmosis, Ion Transport across Membranes and Cellular Energy Transformations, Entropy Production in Biological Systems and its Connection to Metabolic Processes.

### **Block IV: Photochemistry and Transport Phenomenon**

#### **Unit 13: Basics of Photochemistry**

Absorption, Excitation, Photochemical Laws, Quantum Yield, Electronically Excited States, Flash Photolysis, Energy Dissipation by Radiative and Non-Radiative Processes, Absorption Spectra, Franck-Condon Principle, Photochemical Stages-Primary and Secondary Processes.

#### **Unit 14: Properties of Excited States**

Electronically Excited States of Metal Complexes, Charge Transfer Spectra, Photochemical rate law, Kinetics of some important photochemical reactions, Energy Transfer in Photochemical Reactions, Photosensitization and Quenching.

#### **Unit 15: Diffusion and Viscosity**

Diffusion and Viscosity: Transport Phenomenon; Kinetic Theory of Gases; Distribution of Molecular Velocities, Mean Free Path; Diffusion Across Concentration Gradient; Fick's First Law of Diffusion, Relationship between Diffusion Coefficient and Mean Free Path; Viscosity and Coefficient of Viscosity; Osmosis; Diffusion versus Osmosis, Reverse Osmosis, Forward Osmosis

#### **Unit 16: Thermal and Electrical Conduction**

Thermal and Electrical Conduction: Thermal Conduction, Coefficient of Thermal Conductivity and Mean Free Path; Electrical Conduction; Drift Velocity, Relationship between Ionic Mobility and Conductance.

### **Books Recommended/Suggested Readings**

1. Peter Atkins, Julio De Paula, "Physical Chemistry", 9<sup>th</sup> ed., 2010, W. H. Freeman and Company, New York, USA. ISBN 978-1-429-21812-2
2. R. M. O. Mendoza, "Introduction to Chemical Thermodynamics" 2019, Arcler Education Inc. ISBN 978-1774072547
3. N. M. Laurendeau, "Statistical Thermodynamics: Theory and Applications", 1<sup>st</sup> ed., 2005, Cambridge University Press. ISBN 978-0521846356
4. D. Jou, J. C. Vazquez, G. Lebon, "Extended Irreversible Thermodynamics" 4<sup>th</sup> ed. 2009, Springer USA. ISBN 978-9048130733
5. M. Persico, G. Granucci, "Photochemistry: A Modern Theoretical Perspective", Reprint, 2019, Springer USA. ISBN 978-3030079062
6. R. B. Bird, W. E. Stewart, "Transport Phenomena", 2<sup>nd</sup> ed. 2006, Wiley. ISBN 978-8126508082

### **Course Outcomes**

By the end of this course, students will be able to

1. Analyze thermodynamic energy functions (Gibbs, Helmholtz) and chemical potential to predict equilibrium criteria in variable-composition systems.
2. Apply statistical mechanics principles to derive molecular partition functions and calculate thermodynamic properties (entropy, free energy) for ideal gases.
3. Calculate equilibrium constants and reaction rates using partition functions, and relate statistical ensembles to macroscopic thermodynamic potentials.
4. Interpret irreversible thermodynamics through entropy production, Onsager's reciprocity relations, and their applications in non-equilibrium biological systems.
5. Solve photochemical problems involving quantum yield, excited-state kinetics, and energy transfer using photochemical laws and spectroscopic principles.
6. Evaluate transport phenomena (diffusion, viscosity, conduction) through kinetic theory and Fick's/Ohm's laws, linking microscopic behavior to macroscopic properties.
7. Demonstrate the relevance of thermodynamics in biological energy transformations, membrane processes, and metabolic entropy production.

**Course Objectives**

This course aims to provide a thorough understanding of atomic and molecular spectrometric techniques, as well as thermoanalytical methods, enabling students to explore their principles, instrumentation, and real-world applications. Students will analyze spectral data, evaluate analytical parameters (e.g., LOD, LOQ), and apply techniques like FAAS, ICP-AES, UV-Vis, IR, NMR, and DSC to solve chemical problems. Emphasis is placed on integrating theoretical knowledge with practical skills, fostering critical thinking to select and optimize techniques for qualitative and quantitative analysis in diverse scientific contexts.

**Block I: Atomic Spectrometric Techniques****Unit 1: Introduction to Atomic Spectroscopy**

Origin and Classification of Atomic Spectroscopic Methods Atomic Spectrum, Classification of Atomic Spectroscopic Methods; Characteristics of Atomic Spectrum - Position of the Signal, Intensity of the Signal, Spectral Line Width; Principle of Flame Photometry - Fate of the Sample in the Flame; Flame and its Characteristics, Reactions in Flames

**Unit 2: Flame Atomic Absorption Spectrometry (FAAS)**

Principle and Instrumentation, Types of Atomizers: Flame, Electrothermal (Graphite Furnace), Sample Preparation and Introduction Techniques, Sensitivity, Limit of Detection (LOD), Limit of Quantification (LOQ), Working Range, Analytical Applications and Limitations.

**Unit 3: Atomic Emission Spectrometry (AES)**

Principle of Atomic Emission, Types of Emission Sources: Flame, Plasma, Arc and Spark, Instrumentation and Detection Systems, Sensitivity, Limit of Detection (LOD), Limit of Quantification (LOQ), Working Range, Applications in Elemental Analysis.

**Unit 4: Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES)**

Principle and Advantages of ICP as an Excitation Source, Instrumentation: Plasma Torch, RF Generator and Spectrometer, Sample Introduction Methods, Limit of Detection (LOD), Limit of Quantification (LOQ), Working Range, Applications in Multi-Element Analysis.

**Block II: Molecular Spectrometric Techniques-I****Unit 5: Introduction to Molecular Spectroscopy**

Recapitulating EM Radiation and its Characteristics; Interaction of Radiation and Matter, Characteristics of Spectrum; Intensity of Signal; Boltzmann Population Distribution, Einstein Coefficients, Transition Dipole Moments, and Selection Rules; Spectral Width, Natural line Width; S/N Ratio, Computer averaging of transients, Fourier Transform Spectroscopy

**Unit 6: UV-Visible Spectrophotometry**

Principles of UV-Visible Spectroscopy, Electronic Transitions in Molecules:  $\sigma$ - $\sigma^*$ ,  $\pi$ - $\pi^*$ ,  $n$ - $\pi^*$  Transitions, Beer-Lambert Law and its Applications, Instrumentation: Sources, Monochromators, Detectors, Applications in Chemical Analysis and Structure Determination.

**Unit 7: Infrared (IR) Spectrometry**

Principles of IR Spectroscopy, Vibrational Modes of Molecules: Stretching and Bending Vibrations, Selection Rules and Molecular Vibrations, Interpretation of IR Spectra: Functional Group Identification, Instrumentation and Sample Preparation Techniques, Applications in Identifying Functional Groups and Studying Molecular Structure.

**Unit 8: Raman Spectrometry**

Principles of Raman Spectroscopy, Raman Effect and its Origin, Stokes and Anti-Stokes Lines, Instrumentation and Techniques, Comparison of Raman and IR Spectroscopy, Applications in Studying Molecular Vibrations and Structure.

### **Block III: Molecular Spectrometric Techniques-II**

#### **Unit 9: Fluorescence Spectrometry**

Principles of Fluorescence and Phosphorescence, Jablonski Diagram and Electronic Transitions, Quantum Yield and Fluorescence Quenching, Instrumentation and Techniques, Applications in Studying Molecular Environment and Dynamics.

#### **Unit 10: Nuclear Magnetic Resonance Spectrometry (NMR)**

Theory of NMR Spectroscopy - Types of Nuclei, Magnetic Moment, Quantisation, Population of Energy Levels, Larmor Precession, Mechanism of Resonance, Relaxation Mechanisms, Nuclei other than Protons; Fourier Transform NMR; Chemical Shift - Shielding Mechanism, Standard for Chemical Shift, Unit of Chemical Shift, Factors Affecting Chemical Shift; Spin-Spin Coupling - Magnitude of Coupling Constants; Instrumentation for NMR Spectroscopy - Magnet, The Sample Probe, Detector System, Sample Handling, Representation of NMR; Applications of NMR Spectroscopy - Quantitative and Qualitative Applications.

#### **Unit 11: Electron Spin Resonance Spectrometry (ESR)**

ESR Phenomenon; Electron Spin and its Characteristics, Intensity and Representation of ESR Spectrum; Hydrogen atom, Hyperfine Interaction; Isotropic Systems with More Than Two Nuclei, Contributors to Hyperfine Coupling Constants; Anisotropy in g Values; Anisotropy in Hyperfine Coupling

#### **Unit 12: Mass Spectrometry**

Mass Spectrometry: Theory of Mass Spectrometry - Characteristics of Mass Spectrum, Isotopic Peaks; Instrumentation for Mass Spectrometry - Inlet Devices, Ionisation Chamber or Ion Sources, Analysers, Detectors or Ion Collectors, Processing and Output Devices; Applications of Mass Spectrometry - Qualitative Applications of Mass Spectrometry, Quantitative Applications of Mass Spectrometry.

### **Block IV: Thermoanalytical Techniques**

#### **Unit 13: Thermogravimetric Analysis**

Thermogravimetric Analysis: Principle; Instrumentation: Working Function of Each Component; Sources of Error in TGA; Factors Affecting TG Curve; Interpretation of TG Curve Thermogravimetric Analysis (TGA); Application of Thermogravimetric Analysis; Analysis of Inorganic Mixtures, Determination of Nature of Gravimetric Precipitation, Reaction Kinetics

#### **Unit 14: Differential Thermal Analysis**

Differential Thermal Method of Analysis; Principle, Instrumentation, DTA Curves, Factors Affecting DTA Curves, Sources of Errors; Applications of DTA.

#### **Unit 15: Differential Scanning Calorimetry**

Differential Scanning Calorimetry: Experimental Setup, Interpretation of DSC Curve, Applications of DSC, Advantages of DSC.

#### **Unit 16: Isothermal Calorimetry**

Introduction to Isothermal Calorimetry, Thermodynamic Principles, Instrumentation, Modes of Operation: Batch, Flow and Titration Calorimetry, Methodology and Data Analysis, Applications of Isothermal Calorimetry, Challenges and Limitations, Advanced Techniques and Coupled Methods.



### **Books Recommended/Suggested Reading**

1. F. M. Dunnivant, J. W. Ginsbach, "Essential Methods of Instrumental Analysis", 1<sup>st</sup> ed., 2024, John Wiley & Sons Inc. USA. ISBN 978-1394226719
2. D. A. Skoog, F. J. Holler, S. R. Crouch "Principles of Instrumental Analysis", 7<sup>th</sup> ed., 2018, Cengage Learning. ISBN 978-9353506193
3. D. L. Pavia, Lapman, Kriz, Vyvyan, "Introduction to Spectroscopy" 5<sup>th</sup> ed., 2015, Cengage India Privat Ltd. ISBN 978-9381466476
4. N. K. Kaushik, S. K. Shukla, "Thermal Analysis Techniques and Applications, 2023 " TechSar Pvt. Ltd. ISBN 978-9386768735

### **Course Outcomes**

By the end of this course, students will be able to

1. Explain the principles, instrumentation, and applications of atomic spectrometric techniques (FAAS, AES, ICP-AES) for elemental analysis.
2. Interpret molecular spectra (UV-Vis, IR, Raman) to determine functional groups, molecular structure, and electronic transitions.
3. Compare fluorescence, NMR, ESR, and mass spectrometry for studying molecular environments, spin interactions, and isotopic patterns.
4. Evaluate thermoanalytical methods (TGA, DTA, DSC) to assess thermal stability, reaction kinetics, and material properties.
5. Apply analytical parameters (sensitivity, LOD, working range) to assess method performance and troubleshoot experimental limitations.
6. Integrate data from multiple spectroscopic and thermal techniques to address complex analytical challenges in research or industry.

**Course Objectives**

This course aims to provide students with practical knowledge and hands-on experience in analytical and organic chemistry techniques. In analytical chemistry, students will learn colorimetric estimation methods and thin-layer chromatography (TLC) for the identification and separation of compounds. In organic chemistry, students will focus on the extraction and analysis of organic compounds from natural sources, utilizing various methods to isolate and identify bioactive molecules. The course emphasizes developing laboratory skills, understanding chemical properties, and applying theoretical knowledge to real-world scenarios.

**Analytical Chemistry**

1. Colorimetric Estimation of Cr(VI) in Water Samples by Diphenylcarbazide Method.
2. Separation and Identification of Amino Acids in its Mixture by TLC.

**Organic Chemistry**

Extraction and analysis of Organic Compounds from Natural Sources (any four of the following)

1. Isolation of Lycopene from Tomatoes.
2. Isolation of Casein from Milk (The students are required to try some typical colour reactions of proteins).
3. Isolation of Nicotine Dipicrate from Tobacco.
4. Isolation of Piperine from Black Pepper.
5. Isolation of  $\beta$ -Carotene from Carrots.
6. Isolation of Lactose from Milk (Purity of sugar should be checked by TLC and paper chromatography and  $R_F$  values reported).
7. Isolation of Eugenol from Clove.
8. Isolation of Caffeine from Tea leaves – Its Sublimation and TLC.
9. Isolation of (+) Limonine from Citrus Juice or Orange Peel.

**Books Recommended/Suggested Readings**

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry" 5th ed., 2003, Pearson India Ltd. ISBN 9788177589573
2. J. Leonard, B. Lygo, G. Procter "Advanced Practical Organic Chemistry" 3<sup>rd</sup> ed., 2013, CRC Press. ISBN 978-1439860977
3. Daniel. C. Harris, "Quantitative Chemical Analysis" 9th ed., 2015, W. H. Freeman & Co Ltd. ISBN 978-1464135385

**Course Outcomes:**

1. Students will gain hands-on experience in performing colorimetric estimations and thin-layer chromatography, enhancing their ability to analyze and identify compounds accurately.
2. Through the isolation of various organic compounds from natural sources, students will learn essential extraction techniques and methods for analyzing the purity and chemical properties of these compounds.
3. By integrating theoretical principles with practical laboratory skills, students will be able to apply their knowledge to real-world problems, preparing them for advanced research and professional careers in chemistry.

**Course Objectives**

This course is designed to provide M.Sc. Chemistry students with hands-on experience in physical and inorganic chemistry through a series of laboratory experiments. Students will gain practical knowledge in studying reaction kinetics and mechanisms, synthesizing coordination compounds, and analyzing the results to understand chemical processes better. The course aims to enhance students' experimental skills, critical thinking, and ability to compare and interpret data, preparing them for advanced research and professional applications in chemistry.

**Physical Chemistry**

1. Study the saponification of ethyl acetate with sodium hydroxide volumetrically.
2. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate (using both hydrochloric acid and sulphuric acid) titrimetrically. Use this data to compare the strengths of the two acids. Study the reaction at two different temperatures and calculate the thermodynamic parameters.
3. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the Initial Rate Method.
4. Study the kinetics of the iodination of acetone in the presence of acid by the integrated rate equation method.

**Inorganic Chemistry**

Synthesis of the following coordination compounds: (Minimum three experiments will be performed)

1.  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
2.  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
3.  $[\text{Co}(\text{NH}_3)_6] [\text{Co}(\text{NO}_2)_6]$
4.  $\text{TiO} (\text{C}_9\text{H}_8\text{NO})_2\text{H}_2\text{O}$
5.  $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$

**Books Recommended/Suggested Readings**

1. J. N. Gurtu, A. Gurtu, "Advanced Physical Chemistry Experiments", Revised ed., 2008, Pragati Prakashan, Meerut, India. ISBN 978-8183965277
2. N. Gerasimchuk, S. Tyukhtenko, "Inorganic Synthesis: A manual for Laboratory Experiments", 1<sup>st</sup> ed., 2019, Cambridge Scholars Publishing. ISBN 978-1527539204
3. G. S. Girolami, T. B. Rauchfuss, R. J. Angelici, "Synthesis and Technique in Inorganic Chemistry", 3<sup>rd</sup> ed. 1999, University Science Books, USA. ISBN 978-0935702484

**Course Outcomes**

1. Students will develop the ability to conduct precise and accurate experiments in physical and inorganic chemistry, including the synthesis of coordination compounds and the study of reaction kinetics.
2. Students will learn to analyze experimental data critically, compare reaction rates, and calculate thermodynamic parameters, enabling them to understand chemical reactions' underlying mechanisms and factors.
3. The course will prepare students for advanced research by providing a strong foundation in experimental techniques and methodologies, fostering a deeper understanding of physical and inorganic chemistry principles applicable in academic and industrial settings.

## SEMESTER: III

**Course Name: Biophysical and Computational Chemistry**

**Code: CHM-7111**

**Credits: 4**

### **Course Objectives**

This course provides a deep understanding of molecular and biophysical principles driving biological systems, focusing on biomolecular structure, interactions, and dynamics. Students will analyze proteins, nucleic acids, and membranes using thermodynamics, statistical mechanics, and computational tools like molecular docking and AI-driven simulations. The curriculum integrates foundational concepts (enzyme kinetics, biopolymer thermodynamics) with advanced techniques (quantum biochemistry, drug design) to solve real-world challenges in biochemistry, molecular medicine, and biophysics, fostering analytical and innovation skills.

### **Block I: Molecular Basis of Biological Systems**

#### **Unit 1: Biological Cell and its Constituents**

Biological Cell, Structure and Functions of Proteins, Enzymes, DNA and RNA in Living Systems, Helix Coil Transition.

#### **Unit 2: Bioenergetics**

Standard Free Energy Change in Biochemical Reactions, Exergonic, Endergonic. Hydrolysis of ATP, Synthesis of ATP from ADP.

#### **Unit 3: Statistical Mechanics of Biopolymers**

Chain Configuration of Macromolecules, Statistical Distribution End to End Dimensions, Calculation of Average Dimensions for Various Chain Structures, Polypeptide and Protein Structures, Introduction to Protein Folding Problem.

#### **Unit 4: Biopolymer Interactions**

Forces Involved in Biopolymer Interactions, Electrostatic Charges and Molecular Expansion, Hydrophobic Forces, Dispersion Force Interactions, Multiple Equilibria and Various Types of Binding Processes in Biological Systems, Hydrogen Ion Titration Curves.

### **Block II: Biopolymers and Membrane Dynamics**

#### **Unit 5: Thermodynamics of Biopolymer Solutions**

Thermodynamics of Biopolymer Solutions, Osmotic Pressure, Membrane Equilibrium, Muscular Contraction and Energy Generation in Mechanochemical System.

#### **Unit 6: Cell Membrane and Transport of Ions**

Structure and Functions of Cell Membrane, Ion Transport through Cell Membrane, Irreversible Thermodynamic Treatment of Membrane Transport, Nerve Conduction.

#### **Unit 7: Biopolymers and their Molecular Weights**

Evaluation of Size, Shape, Molecular Weight and Extent of Hydration of Biopolymers by Various Experimental Techniques. Sedimentation Equilibrium, Hydrodynamic Methods, Diffusion, Sedimentation Velocity, Viscosity, Electrophoresis and Rotational Motions.

#### **Unit 8: Diffraction Methods**

Light Scattering, Low Angle X-Ray Scattering, X-Ray Diffraction and Photo Correlation Spectroscopy, Optical Rotatory Dispersion (ORD).

### **Block III: Biophysical Applications in Molecular Systems**

#### **Unit 9: Protein-Ligand Interactions**

Thermodynamics and Kinetics of Protein-Ligand Binding, Techniques for Studying Protein-Ligand Interactions: ITC, SPR, and NMR, Binding Affinity and Cooperativity, Molecular Docking

Approaches for Studying Interactions.

**Unit 10: DNA and RNA Interactions**

Structural Aspects of DNA/RNA-Ligand Interactions, Study of DNA Melting and Reannealing using Spectroscopic Methods, Applications of Electrophoretic Mobility Shift Assay (EMSA), Simulation Studies of Nucleic Acid Structures.

**Unit 11: Computational Drug Design**

Structure-Based Drug Design: Docking And Scoring Functions, Ligand-Based Drug Design: QSAR and Pharmacophore Modeling, ADMET Predictions and Toxicity Assessments, Role of Machine Learning in Computational Drug Discovery.

**Unit 12: Biomolecular Simulations**

Molecular Dynamics of Protein Folding and Unfolding, Membrane-Protein Interactions and Lipid Bilayer Simulations, Coarse-Grained Modeling of Biomolecular Systems, Free Energy Calculations: FEP and Thermodynamic Integration.

**Block IV: Advanced Topics in Biophysical and Computational Chemistry**

**Unit 13: Biophysical Chemistry of Enzymes**

Enzyme Kinetics: Michaelis-Menten and Beyond, Single-Molecule Enzymology Techniques, Computational Modeling of Enzyme Catalysis, Role of Cofactors and Inhibitors in Enzymatic Activity.

**Unit 14: Quantum Biochemistry**

Quantum Mechanical Principles Applied to Enzymatic Reactions, Proton Transfer and Tunneling in Biochemical Systems, Hybrid QM/MM Methods for Biological Systems, Case Studies: Quantum Chemistry of Photosynthesis and Nitrogen Fixation.

**Unit 15: Biomolecular Thermodynamics**

Thermodynamic Stability of Macromolecular Assemblies, Unfolding and Refolding of Proteins: Thermodynamic and Kinetic Aspects, Cooperative and Allosteric Transitions in Proteins, Hydration and Solvation Thermodynamics of Biomolecules.

**Unit 16: Frontiers in Biophysical and Computational Chemistry**

Applications of Artificial Intelligence in Molecular Simulations, Advances in Enhanced Sampling Techniques, Computational Modeling of Biomolecular Crowding, Biophysical Studies of Intrinsically Disordered Proteins (IDPs).

**Books Recommended/Suggested Readings**

1. I. Tinoco Jr., K. Sauer, J. C. Wang, J. D. Puglisi "Physical Chemistry: Principles and Applications in Biological Sciences", 5<sup>th</sup> ed., 2012, Pearson Education Ltd. ISBN 978-0136056065
2. C. R. Cantor and P. R. Schimmel "Biophysical Chemistry: Part I: The Conformation of Biological Macromolecules", 1980, W. H. Freeman & Co Ltd. ISBN 978-0716711889
3. C. R. Cantor and P. R. Schimmel, "Biophysical Chemistry: Part II: Techniques for the Study of Biological Structure and Function", 1980, W. H. Freeman & Co Ltd. ISBN 978-0716711902
4. S. M. Bachrach, "Computational Organic Chemistry", 2<sup>nd</sup> ed., 2014, Wiley, USA. ISBN 978-1118291924
5. E. Clementi, "MOTTECC: Modern Techniques in Computational Chemistry", Softcover reprint, 2012, Springer USA. ISBN 978-9401090599

**Course Outcomes**

By the end of this course, students will be able to

1. Analyze the structural and functional roles of proteins, DNA, RNA, and membranes in biological systems using thermodynamic, kinetic, and statistical mechanics principles.

2. Apply experimental techniques (e.g., ITC, electrophoresis, X-ray diffraction) and computational tools (molecular docking, MD simulations) to study biopolymer interactions and dynamics.
3. Evaluate molecular weights, conformations, and hydration of biopolymers through hydrodynamic, spectroscopic, and scattering methods.
4. Design computational drug candidates using structure/ligand-based approaches, QSAR modeling, and ADMET assessments.
5. Interpret enzyme kinetics, protein-ligand binding thermodynamics, and cooperative/allosteric transitions in biological processes.
6. Integrate quantum mechanical principles (e.g., QM/MM) and methods to solve complex biochemical problems like enzyme catalysis or biomolecular crowding.
7. Critically assess emerging trends in biophysics, including enhanced sampling techniques, intrinsically disordered proteins, and biomolecular simulations.

**Course Name: Organometallic Chemistry**

**Code: CHM-7112**

**Credits: 4**

### **Course Objectives**

The course on Organometallic Chemistry aims to provide students with an in-depth understanding of the fundamental concepts, synthesis, structure, bonding, and reactivity of organometallic compounds. It covers key topics such as the 18-electron rule, metal-ligand interactions, reaction mechanisms, and organometallic compounds of transition metals. Emphasis is placed on the applications of organometallic chemistry in catalysis, organic transformations, bioorganometallic chemistry, and photocatalysis. Additionally, the course explores advanced topics like organometallic clusters, multinuclear complexes, and organometallics of lanthanides and actinides, fostering a comprehensive approach to both theoretical and practical aspects of the field.

### **Block I: Fundamental Concepts in Organometallic Chemistry**

#### **Unit 1: The 18-Electron Rule and Hapticity**

18-Electron Rule: Concept and Exceptions, Electron Counting in Organometallic Complexes, Hapticity of Ligands: Definition and Examples, Applications of Hapticity in Organometallic Compounds.

#### **Unit 2: Metal-Carbon Bonds in Organometallic Compounds**

Metal-Carbon Sigma Bonds: Alkyls And Aryls, Metal-Carbon pi Bonds: Alkenes, Alkynes and Arenes, Backbonding in Organometallic Compounds, Structure and Bonding in Metallocenes.

#### **Unit 3: Metal-Ligand Interactions**

Synergic Bonding in Metal-Ligand Systems, Metal-Ligand Multiple Bonding, Role of d-Orbitals in Metal-Ligand Interactions, Comparative Study of Ligands in Organometallic Chemistry.

#### **Unit 4: Organometallic Reaction Mechanisms**

Oxidative Addition and Reductive Elimination, Insertion and Elimination Reactions, Transmetallation and Migratory Insertion, Nucleophilic and Electrophilic Attack on Ligands.

### **Block II: Organometallic Compounds of Transition Metals**

#### **Unit 5: Organometallic Compounds of Chromium and Manganese**

Synthesis, Structure, Bonding and Properties, Applications in Catalysis and Material Science.

#### **Unit 6: Organometallic Compounds of Iron and Nickel**

Synthesis, Structure, Bonding, and Properties, Role in Industrial Catalytic Processes.

#### **Unit 7: Organometallic Compounds of Cobalt and Rhodium**

Synthesis, Structure, Bonding and Properties, Applications in Homogeneous Catalysis and Organic Synthesis.

#### **Unit 8: Organometallic Compounds of Palladium and Platinum**

Synthesis, Structure, Bonding and Properties, Applications in C-C Coupling Reactions (Heck, Suzuki, and Sonogashira Reactions).

### **Block III: Applications of Organometallic Chemistry**

#### **Unit 9: Catalysis by Organometallic Compounds**

Organometallic Catalysis in Organic Synthesis, Hydrogenation, Hydroformylation and Hydrosilylation Reactions, Polymerization Catalysis: Ziegler-Natta and Metallocene Catalysts.

#### **Unit 10: Organometallics in Organic Transformations**

Role of Organometallics in Selective Transformations, Cross-Coupling Reactions and C-H Activation, Carbene and Carbyne Complexes in Organic Synthesis.

#### **Unit 11: Bioorganometallic Chemistry**

Role of Organometallic Compounds in Biological Systems, Medicinal Applications: Anticancer and

Antimicrobial Agents, Metalloenzymes with Organometallic Cofactors.

**Unit 12: Photochemistry and Photocatalysis in Organometallics**

Photoactivation of Organometallic Compounds, Applications in Photocatalysis and Solar Energy Conversion, Mechanistic Studies in Organometallic Photochemistry.

**Block IV: Advanced Organometallic Chemistry**

**Unit 13: Organometallic Clusters and Cage Complexes**

Structure and Bonding in Metal Clusters, Synthesis and Properties of Metal Carbonyl Clusters, Applications of Organometallic Clusters in Catalysis.

**Unit 14: Multinuclear Organometallic Compounds**

Synthesis, Bonding and Properties of Multinuclear Organometallic Complexes, Cooperative Effects in Multinuclear Complexes, Applications in Multi-Electron Catalytic Processes.

**Unit 15: Organometallic Chemistry of Lanthanides and Actinides**

Organometallic Compounds of Lanthanides and Actinides: Synthesis and Properties, Applications in Catalysis and Nuclear Chemistry, Comparative Study with Transition Metal Organometallics.

**Unit 16: Advanced Techniques in Organometallic Chemistry**

Techniques for Studying Organometallic Compounds: X-Ray Crystallography, NMR, and IR Spectroscopy, Applications of Computational Chemistry in Organometallic Studies, Emerging Trends and Green Chemistry Approaches in Organometallic Research.

**Books Recommended / Suggested Readings**

1. M. Bachmann, "Organometallics 1: Complexes with Transition Metal-Carbon  $\sigma$  -Bonds", 1<sup>st</sup> ed., 1994, Oxford University Press. ISBN 978-0198557500
2. M. Bachmann, "Organometallics 2: Complexes with Transition Metal-Carbon  $\pi$  -Bonds", 1<sup>st</sup> ed., 1994, Oxford University Press. ISBN 978-0198558132
3. R. H. Crabtree, "The Organometallic Chemistry of the Transition Metals", 7<sup>th</sup> ed., 2019, Wiley, USA. ISBN 978-1119465881
4. R. Whyman, "Applied Organometallic Chemistry and Catalysis", 1<sup>st</sup> ed., 2001, Oxford University Press UK. ISBN 978-0198559177
5. G. Jaouen, "Bioorganometallic Chemistry - Application in Drug Discovery, Biocatalysis, and Imaging", 1<sup>st</sup> ed., 2015, Wiley-VCH Verlag GmbH. ISBN 978-3527335275

**Course Outcomes**

1. Students will be able to describe the structure, bonding, and properties of organometallic compounds, including those of transition metals, lanthanides, and actinides.
2. Students will gain knowledge of the role of organometallic compounds in catalysis and organic transformations, and will apply these concepts to industrial and bioorganometallic chemistry.
3. Students will understand and analyze various reaction mechanisms in organometallic chemistry, such as oxidative addition, reductive elimination, and migratory insertions.
4. Students will be proficient in the synthesis and properties of complex organometallic clusters, multinuclear compounds, and techniques such as X-ray crystallography, NMR, and IR spectroscopy in organometallic studies.



**Course Name: Heterocyclic Chemistry and Organic Synthesis****Code: CHM-7113****Credits: 4****Objective**

This course aims to empower students with a foundational understanding of organometallic chemistry, exploring the interplay between metals and organic ligands. Students will grasp key concepts like the 18-electron rule, hapticity, and metal-ligand bonding, while examining synthesis, structure, and reactivity of transition metal organometallics. The curriculum bridges theory with real-world applications, including catalysis, organic synthesis, and bioorganometallic systems. Advanced topics like clusters, multinuclear complexes, and green chemistry approaches will foster critical thinking, equipping students to analyze modern research and innovate in industrial or academic settings.

**Block I: Fundamentals and Small-Membered Heterocycles****Unit 1: Introduction, Classification and Nomenclature of Heterocycles**

Introduction to Heterocyclic Chemistry, Basic Structure and Classification of Heterocycles, Nomenclature (Hantzsch-Widman System) Strain, Bond Angle and Torsional Strains in Small Ring Heterocycles, Conformation of Six-Membered Heterocycles: Molecular Geometry, Barrier to Ring Inversion, Pyramidal Inversion and 1,3-Diaxial Interaction, Stereoelectronic Effects: Anomeric And Related Effects.

**Unit 2: Three and Four-Membered Heterocycles**

Three-Membered Heterocycles: Synthesis and Reactions of Aziridines, Oxiranes and Thiiranes, Four-Membered Heterocycles: Synthesis and Reactions of Azetidines, Oxetanes and Thietanes, Benzofused Analogs: Synthesis and Reactions of Benzopyrroles, Benzofurans and Benzothiophenes.

**Unit 3: Five-Membered Heterocycles**

Monocyclic Five-Membered Rings: Synthesis and Reactions of Five-Membered Rings with one Heteroatom (N, O, S), Synthesis and Reactions of Five-Membered Rings with Two Heteroatoms (N, O, S), Benzofused Analogs: Synthesis and Reactions of Benzofused Five-Membered Heterocycles.

**Unit 4: Six-Membered Heterocycles with One Heteroatom**

Pyridine and Analogues: Synthesis and Reactions of Pyridine, Pyrilium Salts and Pyrones, Comparison with Pyridinium and Thiopyrylium Salts and Pyridones, Benzofused Analogues: Synthesis and Reactions of Quinolizinium and Benzopyrylium Salts.

**Block II: Larger and Meso-ionic Heterocycles****Unit 5: Six-Membered Heterocycles with Two or More Heteroatoms**

Diazines: Synthesis and Reactions of Diazines, Benzofused Diazines: Synthesis and Reactions of Benzofused Diazines.

**Unit 6: Meso-Ionic Heterocycles**

Classification: Types and Structural Characteristics of Meso-Ionic Heterocycles, Synthesis and Reactions: Methods of Synthesis and General Reactions of Meso-Ionic Heterocycles.

**Unit 7: Seven-Membered Heterocycles**

Azepines: Synthesis and Reactions of Azepines, Oxepines and Thiepines: Synthesis and Reactions of Oxepines and Thiepines.

**Unit 8: Large-Membered Heterocycles**

Diazepines: Synthesis and Reactions of Diazepines, Thiazepines: Synthesis and Reactions of Thiazepines.

**Block III: Basic Concepts of Organic Synthesis****Unit 9: Philosophy of Organic Synthesis**

Disconnection Approach; One Group and Two Group Disconnections; Reversal of Polarity; Chemoselectivity; One Group C-C Disconnections; Two Group C-C Disconnections; 1,3-difunctional and 1,5-difunctional Compounds; Tandem Reactions, Domino Reactions and Multi-component Reactions

#### **Unit 10: Reductions**

Catalytic Hydrogenation: Stereochemistry and Mechanism; Metal liquid Ammonia Reductions: Stereoselection and Mechanism; Homogeneous Hydrogenations; Mechanisms and Applications Using Rh, Ru and Other Metal Complexes

#### **Unit 11: Reductions using Hydride Transfer Reagents**

Sodium Borohydride; Sodium Cyanoborohydride; Lithium Aluminium Hydride and Alkoxy Substituted LAH Reducing Agents; DIBAL; Applications of Hydroboration (Reductions, Oxidations and Carbonylations); Diborane Coupling Reaction; Diisooamylborane, Thexylborane and 9-BBN; Isopinocampheyl and Diisopinocampheylboranes

#### **Unit 12: Oxidations**

Use of Oxidizing Reagents with Applications and Mechanism; DDQ, SeO<sub>2</sub>, Ti(NO<sub>3</sub>)<sub>3</sub>, Ceric Ammonium Nitrate; Sharpless Asymmetric Epoxidation; Asymmetric Hydroxylation and Aminohydroxylation

### **Block IV: Organic Synthesis: Some More Approaches**

#### **Unit 13: Enolates**

Thermodynamic Versus Kinetic Enolates; Enolate Equivalents and Enamines; Applications in Carbon-Carbon Bond Formation and Related Reactions; Applications in Chiral Synthesis

#### **Unit 14: Umpolung Reactions**

Sulphur Compounds; Nitro Compounds; Lithiated Ethers and Related Compounds

#### **Unit 15: Principles and Applications of Phase Transfer Catalysis**

Crown Ethers; Polymer-Supported Reagents in Organic Synthesis

#### **Unit 16: Asymmetric Synthesis**

Development of Methodologies for Asymmetric Synthesis; Regioselectivity; Stereoselectivity; Diastereoselectivity and Stereospecificity

### **Books Recommended/Suggested Readings**

1. J. A. Joule, K. Mills "Heterocyclic Chemistry", 1<sup>st</sup> ed., 2010, Wiley-Blackwell, USA. ISBN 978-1405133005
2. J. A. Builla, J. J. Vaquero, J. Barluenga, "Modern Heterocyclic Chemistry", 1<sup>st</sup> ed., 2011, Wiley-VCH Verlag GmbH. ISBN 978-3527332014
3. M. B. Smith, "March's Advanced Organic Chemistry: Reactions Mechanisms and Structure", 7<sup>th</sup> ed., 2015, John Wiley & Sons Inc. USA. ISBN 978-8126556588
4. A. Warren, P. Wyatt, "Organic Synthesis: The Disconnection Approach", 2<sup>nd</sup> ed., 2008 Wiley, USA. ISBN 978-0470712368
5. F. A. Carey, R. J. Sundberg, "Advanced Organic Chemistry Part B: Reactions and Synthesis", 5<sup>th</sup> ed., 2007, Springer India Private Ltd. ISBN 978-8132204268

### **Course Outcomes**

By the end of this course, students will be able to

1. Apply the 18-electron rule and hapticity principles to predict stability and bonding in organometallic complexes.

2. Analyze metal-ligand interactions, reaction mechanisms (e.g., oxidative addition, migratory insertion), and their roles in catalytic cycles.
3. Synthesize and characterize organometallic compounds of transition metals (Cr, Fe, Pd, etc.), linking their structures to industrial applications like cross-coupling reactions.
4. Evaluate organometallic catalysts in hydrogenation, polymerization, and photochemical processes, emphasizing sustainability and efficiency.
5. Design strategies using bioorganometallic systems or computational tools to address challenges in medicine, energy, and green chemistry.
6. Critically assess advanced topics such as metal clusters, lanthanide complexes, and emerging trends through case studies and research literature.

**Course Objectives**

This course aims to introduce M.Sc. Chemistry students to the fundamentals of research formulation, design, data analysis, and report writing. It focuses on the essential steps in conducting scientific research, from defining the research problem to presenting findings in a structured report. Key topics include ethical issues, literature review, hypothesis formulation, data analysis using statistical tools, and effective use of computer applications in research. The course will equip students with the necessary skills to conduct high-quality research, ensuring scientific integrity, reproducibility, and adherence to intellectual property rights.

**Block I: Research Formulation**

**Unit 1: Introduction to Research**

Definition, objectives, and significance of research. Characteristics and types of research — basic, applied, and interdisciplinary research.

**Unit 2: Research Process and Defining the Research Problem**

Steps in the research process, formulating a research problem, criteria for research problem selection, and problem identification.

**Unit 3: Review of Literature**

Purpose, sources, methods for literature survey, organizing and writing a review of literature.

**Unit 4: Ethical Issues and Intellectual Property Rights in Research**

Ethical considerations in research and publication, plagiarism detection tools, avoiding unethical practices, reproducibility and transparency in research, intellectual property rights (IPR), and patents.

**Block II: Research Elaborated**

**Unit 5: Objectives and Hypothesis Formulation**

Defining Research Objectives and Hypothesis, Characteristics, Types and Significance.

**Unit 6: Research Design**

Concept and Importance of Research Design, Types of Research Designs — Experimental, Descriptive, Exploratory.

**Unit 7: Concept of Sample and Sampling Techniques**

Population and Sample, Sampling methods — Probability and Non-probability Sampling, Sampling Errors, and Sample Size Determination.

**Unit 8: Types and Methods of Data Collection**

Primary and Secondary Data, Qualitative and Quantitative Data Collection Methods, Designing Questionnaires and Interviews.

**Block III: Data Analysis and Interpretation**

**Unit 9: Processing of Data**

Data Coding, Editing and Tabulation, Handling Missing Data, Classification of Data.

**Unit 10: Charts and Diagrams in Data Analysis**

Visual Representation of Data — Types of Charts and Diagrams, Best Practices in Data Visualization.

**Unit 11: Statistical Tools for Data Analysis**

Measures of Central Tendency and Dispersion, Correlation, Regression, Variance Analysis, Use of Software Tools for Statistical Analysis.

**Unit 12: Hypothesis Testing**

Concepts, Types of Errors, Confidence Intervals, p-Values, Parametric and Non-Parametric Tests.

## **Block IV: Report Writing**

### **Unit 13: Report Writing**

Characteristics, Importance and Stages of Report Writing, Guidelines for Presenting Research Findings.

### **Unit 14: Layout of Research Report**

Title Page, Abstract, Introduction, Methodology, Results, Discussion, Conclusion and References.

### **Unit 15: Preparation of PowerPoint Presentations**

Designing Effective Presentation Slides, Communication Techniques for Research Findings.

### **Unit 16: Computer Applications in Research**

Use of Software Tools for Data Analysis, Reference Management Tools, Word Processing and Spreadsheets for Research.

## **Books Recommended/Suggested Readings**

1. C. R. Kothari, G. Garg, "Research Methodology", 4<sup>th</sup> ed., 2019, New Age International Publishers. ISBN 978-9386649225
2. J. D'Angelo, "Ethics in Science: Ethical Misconduct in Scientific Research", 2<sup>nd</sup> ed., 2018, CRC Press. ISBN 978-1138392441
3. K. Healy, "Data Visualization: A Practical Introduction", 2018, Princeton University Press. ISBN 978-0691181622
4. B. Gastel, R. A. Day, "How to Write and Publish a Scientific Paper", 8<sup>th</sup> ed., 2017, Cambridge University Press. ISBN 978-1316640432

## **Course Outcomes**

1. Students will gain a solid foundation in the research process, including problem definition, literature review, and the importance of ethics in research.
2. Students will develop the ability to formulate research objectives and hypotheses, design research studies, and apply appropriate data collection and analysis methods.
3. Students will be equipped with statistical tools for data analysis and hypothesis testing, enhancing their ability to analyze complex scientific data.
4. Students will learn the structure and formatting of research reports, ensuring they can effectively communicate their research findings while adhering to ethical standards in scientific publication.

**Course Objectives**

This course is designed to provide hands-on experience and a deep understanding of advanced experimental techniques in biophysical and computational chemistry as well as organometallic chemistry. Students will learn to determine thermodynamic parameters, investigate molecular interactions, and perform spectroscopy for biological macromolecules. Additionally, they will gain expertise in computational methods for molecular modeling, energy minimization, and molecular docking. In the organometallic chemistry section, students will synthesize key organometallic compounds and study their structures and reactivities using modern spectroscopic techniques and catalysis methods.

**Biophysical and Computational Chemistry (Minimum three experiments will be performed)**

1. Determination of Thermodynamic Parameters for Micelle Formation Using Conductivity Measurements.
2. Investigation of Hydrogen Bonding Effects in Alcohols via Vapor Pressure Measurements.
3. UV-Visible Spectroscopic Determination of Protein and DNA Concentration and Purity.
4. Fluorescence Quenching Studies of Protein-Ligand Interactions.
5. Energy minimization, geometry optimization and visualization of molecular orbitals of small molecules by DFT.
6. Molecular Docking of Ligands to Proteins Using AutoDock Software.

**Organometallic Chemistry (Minimum three experiments will be performed)**

1. Prepare ferrocene and study its structure using UV-Vis, IR, and NMR spectroscopy.
2. Palladium-Catalyzed Suzuki-Miyaura Coupling Reaction.
3. Catalytic Hydrogenation of an Alkene Using Wilkinson's Catalyst.
4. Ziegler-Natta Polymerization of Ethylene.
5. Prepare a Fischer-type carbene complex and study its reactivity with nucleophiles.

**Books Recommended/Suggested Readings**

1. A. W. Adamson, A. P. Gast "Physical Chemistry of Surfaces", 6<sup>th</sup> ed., 1997, Wiley Interscience. ISBN 978-0471148739
2. D. A. Skoog, F. J. Holler, S. R. Crouch "Principles of Instrumental Analysis", 7<sup>th</sup> ed., 2018, Cengage Learning. ISBN 978-9353506193
3. B. Valeur, "Molecular Fluorescence: Principles and Applications", 2002, Wiley-VCH Verlag GmbH. ISBN 978-3527299195
4. F. Jensen, "Introduction to Computational Chemistry", 3<sup>rd</sup> ed, 2017, Wiley, USA. ISBN 978-1118825990
5. M. Bachmann, "Organometallics 1: Complexes with Transition Metal-Carbon  $\sigma$  -Bonds", 1<sup>st</sup> ed., 1994, Oxford University Press. ISBN 978-0198557500
6. M. Bachmann, "Organometallics 2: Complexes with Transition Metal-Carbon  $\pi$  -Bonds", 1<sup>st</sup> ed., 1994, Oxford University Press. ISBN 978-0198558132
7. R. H. Crabtree, "The Organometallic Chemistry of the Transition Metals", 7<sup>th</sup> ed., 2019, Wiley, USA. ISBN 978-1119465881

**Course Outcomes**

1. Students will acquire practical skills in using advanced experimental techniques to investigate

thermodynamic parameters, molecular interactions, and the structural properties of biological macromolecules.

2. Students will gain proficiency in computational chemistry techniques, including energy minimization, geometry optimization, and molecular docking, and apply these methods to solve chemical problems.
3. Students will be able to synthesize and characterize key organometallic compounds, understand their reactivities, and apply this knowledge to catalysis and material science applications.

**Course Objectives**

The objective of this course is to provide students with an in-depth understanding of the synthesis and characterization of heterocyclic compounds, and the application of spectroscopic techniques in determining the structure and reactivity of organic molecules. Students will learn practical methods for synthesizing various heterocycles and will be trained in the use of IR, NMR, UV, and mass spectrometry to analyze and interpret complex spectral data, enabling them to deduce the structures and properties of organic compounds.

**Heterocyclic Chemistry and Organic Synthesis**

1. Synthesis of Benzofuran from Salicylaldehyde and Ethyl Bromide Using Phase Transfer Catalysis.
2. Synthesis of Aziridine from Ethanolamine and Characterization by IR and NMR Spectroscopy.
3. Synthesis of Diazine Derivatives Using Condensation Reactions. (Minimum two).
4. Preparation of Meso-ionic 1,3-Oxazolium-5-olate and Study of Its Reactivity Using Kinetic Methods.
5. Reduction of a Carbonyl Compound using Lithium Aluminum Hydride (LAH).
6. Synthesis of an  $\alpha,\beta$ -Unsaturated Carbonyl Compound via Enolate Chemistry.
7. Asymmetric Epoxidation of an Alkene using Sharpless Epoxidation.

**Books Recommended/Suggested Readings**

1. J. A. Joule, K. Mills "Heterocyclic Chemistry", 1<sup>st</sup> ed., 2010, Wiley-Blackwell, USA. ISBN 978-1405133005
2. J. A. Builla, J. J. Vaquero, J. Barluenga, "Modern Heterocyclic Chemistry", 1<sup>st</sup> ed., 2011, Wiley-VCH Verlag GmbH. ISBN 978-3527332014
3. M. B. Smith, "March's Advanced Organic Chemistry: Reactions Mechanisms and Structure", 7<sup>th</sup> ed., 2015, John Wiley & Sons Inc. USA. ISBN 978-8126556588
4. A. Warren, P. Wyatt, "Organic Synthesis: The Disconnection Approach", 2<sup>nd</sup> ed., 2008 Wiley, USA. ISBN 978-0470712368
5. R. Noyori, "Asymmetric Catalysis in Organic Synthesis", 1<sup>st</sup> ed., 1994, John Wiley & Sons Inc. ISBN 978-0471572671

**Course Outcomes**

1. Students will acquire the ability to synthesize a range of heterocyclic compounds using various synthetic methods and phase transfer catalysis, and characterize them using IR and NMR spectroscopy.
2. Students will develop proficiency in analyzing and interpreting UV, IR, NMR, and mass spectra to determine the structures of organic compounds, understand fragmentation patterns, and identify molecular ion peaks.
3. Students will gain practical experience in studying the reactivity of meso-ionic compounds using kinetic methods, enhancing their understanding of reaction mechanisms and the dynamic behavior of organic molecules.



## SEMESTER: IV

**Course Name: Green Chemistry**

**Code: CHM-7211**

**Credits: 2**

### **Course Objectives**

This course aims to provide a foundational understanding of green chemistry principles and their role in advancing sustainable development. By exploring innovative synthesis methods, solvent-free reactions, and catalytic processes, students will examine how chemical processes can minimize environmental harm while maximizing efficiency. Through case studies and industrial applications, the course emphasizes designing eco-friendly materials, optimizing resource use, and addressing global challenges like pollution and climate change. Students will critically evaluate emerging trends, fostering the ability to integrate green chemistry into research, industry, and policy for a safer, sustainable future.

### **Block I: Green Chemistry and Sustainability**

#### **Unit 1: Introduction to Green Chemistry**

Green chemistry: History, Need and Goals, Basic Principles of Green Chemistry, Illustrations of the Principles with Examples.

#### **Unit 2: Introduction to Sustainability**

Definitions, Dimensions of sustainability, Sustainable Development Goals (SDGs) Limitations/obstacles in pursuing the Goals, Opportunities for Materials Designers to Create a Safer Future.

#### **Unit 3: Green Synthesis Methods**

Green Starting Materials and Reagents, Green Solvents and Reaction Conditions, Evolution of the Reaction Type: Rearrangements (100% Atom Economic), Addition Reactions (100% Atom Economic), Non-Conventional Energy-Assisted Reactions: Microwave-Assisted Reactions, Ultrasound-Assisted Reactions, Photochemical Reactions Using Sunlight.

#### **Unit 4: Green Solvents and Reaction Media**

Green Solvents and Aqueous Media, Enhancing Selectivity, Efficiency and Industrial Applicability, Ionic Liquids and their Role in Green Chemistry, Supercritical Fluids in Green Chemistry.

### **Block II: Advances and Applications in Green Chemistry**

#### **Unit 5: Solvent-Free Reactions**

Solvent-Free Reactions in the Liquid Phase, Solvent-Free Reactions in the Solid Phase, Role of Non-Conventional Energy Sources.

#### **Unit 6: Catalysis in Green Chemistry**

Characteristics of Catalysts, Catalysts Affecting Energy Usage and Reagent Stoichiometry, Zeolites for Solid Acid Catalysis, Biocatalysis in Green Synthesis: Catechol Synthesis, Baeyer-Villiger Oxidation, Molecular vs. Enzymatic Catalysis.

#### **Unit 7: Future Trends in Green Chemistry**

Emerging Oxidation-Reduction Reagents and Catalysts, Biomimetic and Multifunctional Reagents, Combinatorial Green Chemistry Approaches, Innovations in Solvent-Less Reactions.

#### **Unit 8: Green Chemistry in Industry and Environment**

Proliferation of Solvent-Less Reactions, Noncovalent Derivatization, Biomass Conversion and Utilization, Emission Control Strategies in Chemical Processes, Hazard Assessment and Mitigation in the Chemical Industry.

**Books Recommended/Suggested Reading**

1. M. Lancaster, "Green Chemistry: An Introductory Text", 2<sup>nd</sup> ed., 2010, Royal Society of Chemistry. ISBN 978-1847558732
2. P. T. Anastas, J. C. Warner, "Green Chemistry: Theory and Practice", Reprint, 2005, Oxford University Press, UK. ISBN 978-0198506980
3. R. A. Sheldon, I. Arends, U. Hanefeld, "Green Chemistry and Catalysis", 2006, Wiley-VCH Verlag GmbH. ISBN 978-3527611003
4. S. K. Sharma, A. Mudhoo, "Green Chemistry for Environmental Sustainability", 2019, CRC Press. ISBN 978-1032297903

**Course Outcomes**

On successful completion of this course, students shall be able to

1. Analyze the principles of green chemistry and sustainability to propose solutions aligned with the UN Sustainable Development Goals (SDGs).
2. Design atom-efficient reactions using non-conventional energy sources (microwave, ultrasound) and green solvents (ionic liquids, supercritical fluids).
3. Evaluate the role of catalysts (zeolites, enzymes) in reducing energy consumption and waste generation during chemical synthesis.
4. Propose solvent-free reaction strategies and assess their industrial applicability for minimizing environmental footprints.
5. Develop mitigation strategies for hazards in chemical industries by integrating biomass conversion, emission control, and green process innovations.

## Programme Elective - I

**Course Name: Supramolecular Chemistry**

**Code: CHM-7212**

**Credits: 4**

### **Course Objectives**

This course aims to provide a foundational understanding of supramolecular chemistry, focusing on non-covalent interactions, molecular recognition, and self-assembly principles. Students will critically analyze the thermodynamics, kinetics, and design strategies behind host-guest systems, supramolecular polymers, and molecular devices. Through interdisciplinary exploration, students will connect theory to real-world applications in catalysis, nanotechnology, drug delivery, and sustainable materials. The course emphasizes problem-solving, innovation, and the ability to evaluate emerging trends, preparing learners to address challenges in biomedicine, energy, and environmental science using supramolecular approaches.

### **Block I: Fundamentals and Principles of Supramolecular Chemistry**

#### **Unit 1: Introduction to Supramolecular Chemistry**

Definition and Historical Development, Key Concepts: Host-Guest Chemistry, Molecular Recognition, and Self-Assembly, Non-Covalent Interactions: Hydrogen Bonding, Van der Waals Forces,  $\pi$ - $\pi$  Interactions and Electrostatic Interactions, Importance and Applications in Chemistry and Biology.

#### **Unit 2: Thermodynamics and Kinetics of Supramolecular Systems**

Binding Constants and Cooperative Binding, Entropy and Enthalpy in Supramolecular Interactions, Kinetics of Host-Guest Complexation and Methods for Studying Supramolecular Interactions (UV-Vis, NMR, ITC).

#### **Unit 3: Molecular Recognition and Selectivity**

Mechanisms of Molecular Recognition, Concepts of Complementarity and Preorganization, Selectivity in Host-Guest Chemistry, Role of Solvent and Environmental Factors in Recognition.

#### **Unit 4: Self-Assembly and Self-Organization**

Principles of Molecular Self-Assembly, Dynamic Covalent Chemistry in Self-Organization, Hierarchical Self-Assembly: From Molecules to Materials, Applications in Nanotechnology and Material Science.

### **Block II: Host-Guest Chemistry and Molecular Devices**

#### **Unit 5: Host Molecules and Their Synthesis**

Design and Synthesis of Crown Ethers, Cryptands and Calixarenes, Synthesis of Cyclodextrins and Cavitands, Properties and Applications of Synthetic Host Molecules.

#### **Unit 6: Supramolecular Catalysis**

Catalysis within Host-Guest Complexes, Mechanistic Insights into Supramolecular Catalysis, Applications in Organic Synthesis and Green Chemistry.

#### **Unit 7: Supramolecular Polymers and Gels**

Supramolecular Polymers: Synthesis, Structure and Properties, Gel Formation and Characterization, Applications in Drug Delivery and Responsive Materials.

#### **Unit 8: Molecular Machines and Devices**

Rotaxanes and Catenanes: Synthesis and Properties, Molecular Motors and Switches, Supramolecular Devices for Energy Conversion and Storage.

### **Block III: Advanced Topics in Supramolecular Chemistry**

**Unit 9: Anion and Cation Recognition**

Design of Receptors for Anions and Cations, Mechanisms of Recognition and Sensing, Applications in Environmental Monitoring and Biomedical Science.

**Unit 10: Supramolecular Chemistry in Biology**

Supramolecular Interactions in Biological Systems, DNA and RNA Recognition by Synthetic Receptors, Supramolecular Mimicry of Enzyme Functions.

**Unit 11: Supramolecular Chemistry of Fullerenes and Carbon Nanomaterials**

Host-Guest Chemistry of Fullerenes, Supramolecular Interactions with Graphene and Carbon Nanotubes, Applications in Photovoltaics and Nanomedicine.

**Unit 12: Supramolecular Photochemistry**

Photoinduced Processes in Supramolecular Systems, Energy and Electron Transfer in Host-Guest Complexes, Applications in Artificial Photosynthesis and Light-Harvesting Systems.

**Block IV: Applications and Emerging Trends in Supramolecular Chemistry****Unit 13: Supramolecular Chemistry in Drug Delivery**

Mechanisms of Drug Encapsulation and Release, Host-Guest Systems for Targeted Drug Delivery, Supramolecular Hydrogels and Their Biomedical Applications.

**Unit 14: Supramolecular Materials**

Liquid Crystals, Supramolecular Polymers and Gels, Supramolecular Approaches to Porous Materials and MOFs, Applications in Gas Storage, Separation and Catalysis.

**Unit 15: Supramolecular Sensors**

Design Principles for Chemical Sensors, Sensing of Ions, Small Molecules and Biomolecules, Applications in Diagnostics and Environmental Analysis.

**Unit 16: Emerging Trends in Supramolecular Chemistry**

Dynamic Combinatorial Chemistry, Supramolecular systems in Green Chemistry, Advances in Supramolecular Nanotechnology and Biomedicine.

**Books Recommended/Suggested Readings**

1. J. W. Steed, J. L. Atwood, "Supramolecular Chemistry", 3<sup>rd</sup> ed., 2022, Wiley, USA. ISBN 978-1119582519.
2. J. B. Baruah, "Principles and Application of Supramolecular Catalysis", 1<sup>st</sup> ed., 2019, CRC Press Ltd. ISBN 978-0367111649
3. P. J. Cragg, "Supramolecular Chemistry: From Biological Inspiration to Biomedical Applications", 2010, Springer, USA. ISBN 978-9048125814
4. J. X. J. Zhang, K. Hoshino, "Molecular Sensors and Nanodevices", 2019, Elsevier USA. ISBN 978-0128148624

**Course Outcomes**

By the end of this course, students will be able to

1. Analyze the role of non-covalent interactions (hydrogen bonding,  $\pi$ - $\pi$ , electrostatic) in molecular recognition and self-assembly processes.
2. Design synthetic host molecules (e.g., crown ethers, cyclodextrins) and evaluate their applications in catalysis, sensing, and drug delivery.
3. Create strategies to address environmental or biomedical challenges using supramolecular materials (MOFs, hydrogels) and dynamic combinatorial chemistry.
4. Assess emerging trends (green chemistry, nanomedicine) to propose innovative solutions in supramolecular research and technology development.

## Programme Elective - II

**Course Name: Materials Chemistry**

**Code: CHM-7213**

**Credits: 4**

### **Course Objectives**

This course aims to explore the chemistry, design, and application of advanced materials, bridging fundamental principles with real-world innovation. Students will gain a deep understanding of structure-property relationships in glasses, ceramics, composites, and energy materials (batteries, solar cells, fuel cells), while uncovering the transformative potential of smart materials like conducting polymers, hydrogels, and stimuli-responsive systems. Through hands-on insights into characterization techniques (SEM, TEM, XRD) and discussions on cutting-edge topics (high-T<sub>c</sub> superconductors, nonlinear optics), you will develop the skills to critically evaluate materials for healthcare, energy, electronics, and sustainability challenges, fostering problem-solving in interdisciplinary contexts.

### **Block I: Chemistry of Materials**

#### **Unit 1: Introduction to Materials**

Overview of materials science: Types of materials; Structure-property relationships; interdisciplinary nature of materials chemistry, Environment and Healthcare, Historical Development and Future Trends in Materials Science.

#### **Unit 2: Glasses, Ceramics and Composites**

Glasses; Glassy State, Glass Formers and Glass Modifiers, Ceramics: Structure, Properties and Classification of Ceramics; Composites; Classification and formation of Composites; Applications of Glasses, Ceramics and Composites.

#### **Unit 3: Materials for Energy Storage**

Batteries: Lithium-Ion and Solid-State Batteries; Supercapacitors: Materials for Energy Storage and Charge-Discharge Mechanisms;

#### **Unit 4: Materials for Energy Conversion**

Fuel Cells; Principles of Energy Conversion; Materials for Fuel Cell Applications; Solar Cells: Photovoltaic Materials, Organic Solar Cells and Perovskite Solar Cells.

### **Block II: Smart Materials**

#### **Unit 5: Conducting Polymers**

Discovery and Structural Features of Conducting Polymers, Origin of Conductivity in Conducting Polymers, Doping; Mechanism of Conduction; Band Theory, Charge Carriers (Polaron, Bipolaron, Soliton), SSH Solution Theory, Applications of Conducting Polymers; Biosensors, Drug Delivery

#### **Unit 6: Stimuli Sensitive Polymers**

Stimuli Responsive Polymers and their Classification; pH Responsive Smart Polymers; Classification, Mechanism of Action and Applications. Temperature-Responsive Smart Polymers; Factors Affecting Temperature-Responsive behaviour, Mechanism of Action and applications

#### **Unit 7: Hydrogels**

Hydrogels: Introduction and Classification, Polymers Used in Hydrogels, Swelling Characteristics of Hydrogels; Synthesis of Hydrogels; Characterisation of Hydrogels; Biomedical Applications of Hydrogels.

#### **Unit 8: Surface Active Agents**

Surfactants and their Classification; Micelles; CMC and Factors Affecting It; Solubilization by Surfactants and Factors Affecting it; Emulsions, Stabilization of Macroemulsions

### **Block III: Materials for Electronics and Optical Applications**

#### **Unit 9: Thin Films and Langmuir -Blodgett Films**

Preparation Techniques; Evaporation/Sputtering, Chemical Processes, MOCVD, Sol-Gel Etc. Langmuir-Blodgett (LB) Film, Growth Techniques, Photolithography, Properties and Applications of Thin and LB Films.

#### **Unit 10: Ionic Conductors**

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

#### **Unit 11: High $T_c$ Materials**

Defect Perovskites, High  $T_c$  Superconductivity in Cuprates, Preparation and Characterization of 1-2-3 and 2-1-4 Materials, Normal State Properties; Anisotropy; Temperature Dependence of Electrical Resistance; Optical Phonon Modes, Superconducting State; Heat Capacity; Coherence Length, Elastic Constants, Position Lifetimes, Microwave Absorption-Pairing and Multigap Structure in High  $T_c$  Materials, Applications of High  $T_c$  Materials.

#### **Unit 12: Nonlinear Optical Materials**

Nonlinear Optical Materials: Nonlinear Optical Effects, Second and Third Order Molecular Hyperpolarisability, Second Order Electric Susceptibility Materials for Second and Third Harmonic Generation.

### **Block IV: Material Characterisation Techniques**

#### **Unit 13: Scanning electron microscopy (SEM)**

Introduction of Scanning Electron Microscopy (SEM), Basic Principles, Instrumentation and Sample Preparation, Applications of SEM.

#### **Unit 14: Transmission electron microscopy (TEM)**

Introduction to Transmission Electron Microscopy (TEM), Basic Principles, Electron Gun, Electromagnetic Lenses, Imaging, Operating Parameters- Magnification, Resolution, Depth of Field, Applications of TEM.

#### **Unit 15: Energy Dispersive X-ray Spectroscopy (EDS)**

Energy Dispersive X-Ray Spectroscopy (EDS): Introduction of EDS, Basic Principles, Instrumentation and Sample Preparation, Interpretation and Applications of EDS.

#### **Unit 16: Single Crystal X-ray Diffraction (SC-XRD)**

Introduction to X-Ray Diffraction, X-Ray Diffraction from a Single Crystal: Principles, Instrumentation, Data Collection and Processing, Applications of Single Crystal X-Ray Diffraction, Limitations and Challenges in Single Crystal X-Ray Diffraction.

### **Books Recommended/Suggested Readings**

1. W. D. Callister, D. G. Rethwisch, "Materials Science and Engineering: An Introduction", 10<sup>th</sup> ed., 2020, Wiley USA. ISBN 978-1119721772
2. W. D. Kingery, H. K. Bowen, Uhlman, "Introduction to Ceramics", 2<sup>nd</sup> ed., 2012, Wiley India Pvt. Ltd. ISBN 978-8126539994
3. K. K. Chawla, "Composite Materials: Science and Engineering", Reprint, 2016, Springer, USA. ISBN 978-1493950157
4. J. R. Reynolds, B. C. Thompson, T. A. Skotheim, "Handbook of Conducting Polymers", 4<sup>th</sup> ed., 2019, CRC Press. ISBN 978-1138065512
5. I. Galaev, B Mattiasson, "Smart Polymers: Application in Biotechnology and Biomedicine, 2<sup>nd</sup> ed., 2007, CRC Press. ISBN 978-0849391613

6. B. D. Fahlman, "Materials Chemistry", 3<sup>rd</sup> ed., 2018, Springer USA. ISBN 978-9402416381.
7. D. A. Skoog, F. J. Holler, S. R. Crouch "Principes of Instrumental Analysis", 7<sup>th</sup> ed., 2018, Cengage Learning. ISBN 978-9353506193

### **Course Outcomes**

On successful completion of this course, students will be able to

1. Analyze the structure-property relationships of glasses, ceramics, composites, and energy materials to propose solutions for storage/conversion challenges.
2. Design smart material systems (e.g., stimuli-responsive polymers, hydrogels) for applications in biosensing, drug delivery, and environmental sustainability.
3. Evaluate electronic and optical materials (thin films, ionic conductors, superconductors) for advancements in device engineering and energy efficiency.
4. Apply characterization techniques (SEM, TEM, EDS, XRD) to interpret material behavior and validate performance in research or industrial settings.
5. Critique the role of materials chemistry in addressing global issues, from healthcare innovations to sustainable energy transitions.

## Programme Elective - III

**Course Name: Chemistry of Natural Products**

**Code: CHM-7214**

**Credits: 4**

### **Course Objectives**

This course aims to empower students with a comprehensive understanding of natural products, their chemical diversity, and their pivotal role in drug discovery and sustainable science. Through an exploration of biosynthesis, classification, and analytical techniques, students will connect the dots between plant, marine, and microbial metabolites and their pharmacological applications. The curriculum nurtures critical thinking by integrating traditional knowledge with modern analytical tools like NMR and LC-MS, while emphasizing green chemistry principles. By the end, students will appreciate the synergy of natural product chemistry in addressing global health challenges and advancing eco-friendly scientific practices.

### **Block I: Introduction to Natural Products**

#### **Unit 1: Classification and General Aspects**

Definition and Classification of Natural Products, Primary and Secondary Metabolites, Sources of Natural Products: Plants, Microorganisms and Marine Organisms, Importance of Natural Products in Drug Discovery and Development.

#### **Unit 2: Biosynthesis of Natural Products**

General Pathways: Shikimic Acid, Mevalonic Acid and Acetate Pathways, Enzyme-Catalyzed Reactions in Biosynthesis, Precursor-Product Relationships.

#### **Unit 3: Alkaloids**

Classification, Occurrence and Functions of Alkaloids, Structure, Biosynthesis and Medicinal Applications of Important Alkaloids: Morphine, Quinine and Atropine, Isolation and Purification Techniques.

#### **Unit 4: Terpenoids and Steroids**

Classification, Structure and Biosynthesis of Terpenoids, Monoterpenes, Sesquiterpenes, Diterpenes, and Triterpenes, Steroids: Structure, Synthesis, and Biological Importance of Cholesterol and Hormones.

### **Block II: Chemistry of Carbohydrates, Lipids, and Phenolics**

#### **Unit 5: Carbohydrates**

Classification and Structural Features of Carbohydrates, Reactions of Monosaccharides, Disaccharides and Polysaccharides, Applications in Natural Product Chemistry and Drug Design.

#### **Unit 6: Lipids**

Classification and Biological Importance of Lipids, Fatty Acids, Glycerides, Phospholipids and Sphingolipids, Biosynthesis and Degradation of Lipids. Chemistry, Biosynthesis and Biological Functions of Prostaglandins, Role of Eicosanoids in Inflammation and Signaling Pathways, Applications in Therapeutics and Diagnostics.

#### **Unit 7: Phenolic Compounds**

Classification, Occurrence and Properties of Phenolics, Biosynthesis and Chemical Reactivity of Flavonoids, Tannins and Lignins, Role of Phenolics in Plants and their Pharmacological Applications.

#### **Unit 8: Proteins**

Introduction to Proteins, Protein structure: Primary, Secondary, Tertiary and Quaternary, Protein Folding and Stability: Thermodynamics and Pathways, Structure Function Relationships, Methods of Structural Determination and Proteins in Complex Biological Systems.



### **Block III: Biochemical and Analytical Aspects**

#### **Unit 9: Vitamins and Coenzymes**

Classification and Chemical Structure of Vitamins, Water-Soluble and Fat-Soluble Vitamins: Functions and Deficiency Diseases, Coenzyme Chemistry: Role in Metabolic Reactions.

#### **Unit 10: Enzymes**

Structure and Function of Enzymes, Mechanisms of Enzyme Action, Role of Enzymes in Natural Product Biosynthesis.

#### **Unit 11: Antibiotics**

Classification and Mode of Action of Antibiotics, Structure and Biological Activity of Penicillins, Tetracyclines and Streptomycins, Development of Resistance and Strategies to Overcome It.

#### **Unit 12: Isolation and Purification of Natural Products**

Extraction and Purification Methods, Chromatographic Techniques for the Analysis of Natural Products, Hyphenated Techniques: GC-MS, LC-MS and CE-MS for Complex Natural Product Mixtures.

#### **Unit 13: Structure Elucidation Tools and Strategies**

HRMS (High-Resolution Mass Spectrometry) and 2D-NMR, Circular Dichroism (CD) and Optical Rotatory Dispersion (ORD) for Stereochemical Analysis, X-Ray Crystallography: Role in Determining the 3D Structure of Natural Products

### **Block IV: Natural Products in Different Domains**

#### **Unit 14: Marine Natural Products**

Unique Features of Marine Natural Products, Structure, Biosynthesis and Applications of Marine Alkaloids, Terpenoids and Polyketides, Challenges in Studying Marine Natural Products.

#### **Unit 15: Polyketides**

Structure, Biosynthesis and Biological Significance of Polyketides, Examples of Macrolides and Aromatic Polyketides, Applications in Pharmaceuticals and Agriculture.

#### **Unit 16: Natural Products in Drug Development**

Semi-Synthetic Modifications of Natural Products, Case Studies: Taxol, Artemisinin and Epothilones.

#### **Unit 17: Green Chemistry and Natural Products**

Role of Green Chemistry in Natural Product Extraction and Synthesis, Biocatalysis in Natural Product Chemistry, Sustainable Approaches in the Utilization of Natural Resources.

### **Books Recommended/Suggested Readings**

1. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope, J. b. Harborne, "Natural Products: Their Chemistry and Biological Significance", 1<sup>st</sup> ed., 1994, Longman Group UK Limited. ISBN 978-0582060098
2. P. M. Dewick, "Medicinal Natural Products: A Biosynthetic Approach", 3<sup>rd</sup> ed., 2009, John Wiley & Sons Inc. ISBN 978-0470741689
3. J. F. Robyt, "Essentials of Carbohydrate Chemistry", 1998, Springer-Verlag New York Inc. ISBN 978-0387949512
4. J. M. Berg, G. J. Gatto Jr., J. K. Hines, J. L. Tymockzko, L Stryer, "Biochemistry", 10<sup>th</sup> ed., 2023, W. H. Freeman & Co Ltd. ISBN 978-1319498504
5. K. C. Nicolaou, E. J. Sorensen, "Classics in Total Synthesis: Target, Strategies, Methods, 1<sup>st</sup> ed., 1996, Wiley-VCH Verlag GmbH. ISBN 978-3527292318

### **Course Outcomes**

By the end of this course, students will be able to

1. Analyze the chemical diversity and biosynthetic pathways (shikimic acid, mevalonic acid) of natural products, linking their structural features to biological functions.

2. Apply chromatographic, spectroscopic (HRMS, 2D-NMR), and computational tools to isolate, purify, and elucidate complex natural product structures.
3. Evaluate the therapeutic potential of alkaloids, terpenoids, antibiotics, and marine-derived compounds in drug development through case studies like Taxol and artemisinin.
4. Integrate green chemistry principles and biocatalysis into sustainable extraction, synthesis, and utilization of natural resources.
5. Design strategies to address challenges in natural product research, including antibiotic resistance and marine biodiversity exploration.

## Programme Elective - IV

**Course Name: Polymers Chemistry**

**Code: CHM-7215**

**Credits: 4**

### **Course Objectives**

This course offers a comprehensive exploration of polymer chemistry, blending foundational concepts with advanced applications. Students will gain a deep understanding of polymerization mechanisms, structure-property relationships, and cutting-edge synthesis techniques. They will learn to characterize polymers using modern analytical tools and evaluate their applications in industries like healthcare, energy, and electronics. Emphasizing sustainability, the course encourages critical thinking about biodegradable materials, recycling, and emerging trends such as smart polymers. By bridging theory with real-world challenges, learners will develop the skills to innovate in material design and address global environmental and technological needs.

### **Block I: Fundamentals and Synthesis of Polymers**

#### **Unit 1: Introduction to Polymers**

Definition and Classification of Polymers, Structure and Properties of Polymers: Linear, Branched, and Cross-Linked, Concept of Molecular Weight in Polymers: Number Average and Weight-Average Molecular Weight, Polydispersity Index, Natural and Synthetic Polymers: General Overview.

#### **Unit 2: Mechanism of Polymerization**

Step-Growth Polymerization and Chain-Growth Polymerization, Radical, Cationic and Anionic Polymerization, Coordination Polymerization: Ziegler-Natta Catalysts, Ring-Opening and Condensation Polymerization.

#### **Unit 3: Copolymerization**

Types of Copolymers: Random, Block, Alternating and Graft, Copolymerization Mechanism and Kinetics, Reactivity Ratios and The Concept of Azeotropic Copolymerization, Applications of Copolymers in Industry.

#### **Unit 4: Advanced Polymerization Techniques**

Living Polymerization: ATRP, RAFT and NMP Techniques, Emulsion and Suspension Polymerization, Sol-Gel Polymerization, Solid-State Polymerization Methods.

### **Block II: Properties and Characterization of Polymers**

#### **Unit 5: Physical Properties of Polymers**

Thermal Properties: Glass Transition Temperature ( $T_g$ ) And Melting Temperature ( $T_m$ ), Crystallinity and Factors Affecting Crystallinity in Polymers, Mechanical Properties: Tensile Strength, Elasticity, and Toughness, Electrical and Optical Properties of Polymers.

#### **Unit 6: Chemical Properties of Polymers**

Chemical Stability and Degradation, Polymer Resistance to Solvents, Acids and Bases, Aging and Weathering of Polymers, Additives and Stabilizers in Polymers.

#### **Unit 7: Rheology and Morphology of Polymers**

Viscosity and Viscoelastic Behavior of Polymers, Morphological Analysis of Polymers: Phase Separation and Compatibility, Stress-Strain Relationships and Creep Behavior, Molecular Dynamics in Polymers.

#### **Unit 8: Techniques for Polymer Characterization**

Molecular Weight Determination: GPC and Osmometry, Microscopic Techniques, Spectroscopic Techniques, Dynamic Mechanical Analysis (DMA), Dielectric and Conductivity Studies.

### **Block III: Applications of Polymers**

#### **Unit 9: Polymers in Industry**

Polymers in Packaging, Textiles and Construction, Elastomers and their Industrial Applications,

Thermosets and Thermoplastics in Engineering, Biodegradable and Bio-Based Polymers in Sustainable Industries.

**Unit 10: Polymers in Electronics and Optics**

Conducting Polymers and their Applications, Polymers in LED and OLED Technologies, Photoresponsive and Piezoelectric Polymers, Optical Fibers and Waveguides Using Polymers.

**Unit 11: Biomedical Applications of Polymers**

Polymers in Drug Delivery Systems, Hydrogels and Tissue Engineering Scaffolds, Biopolymers in Medical Implants and Devices, Smart Polymers in Healthcare and Diagnostics.

**Unit 12: Polymers in Energy and Environment**

Polymers in Fuel Cells and Batteries, Polymers in Solar Cell Applications, Polymer Membranes for Water Purification, Recycling and Environmental Impact of Polymers.

**Block IV: Advanced Topics in Polymer Chemistry**

**Unit 13: Polymer Blends and Composites**

Definition and Classification of Polymer Blends and Composites, Miscibility and Phase Behavior in Blends, Fiber-Reinforced and Particulate Composites, Applications in Aerospace and Automotive Industries.

**Unit 14: Nanopolymers and Smart Polymers**

Nanostructured Polymers: Synthesis and Properties, Stimuli-Responsive Polymers: Thermal, Ph, and Light-Sensitive, Polymers in Nanomedicine and Nanotechnology, Functionalization and Applications of Smart Polymers.

**Unit 15: Biopolymers and Sustainable Polymers**

Structure and Properties of Natural Polymers: Starch, Cellulose and Chitosan, Biodegradable Synthetic Polymers, Polymers from Renewable Resources, Challenges and Advancements in Sustainable Polymer Development.

**Unit 16: Emerging Trends in Polymer Research**

Polymers in Additive Manufacturing (3D Printing), Self-Healing and Recyclable Polymers, Supramolecular Polymers: Synthesis and Applications, Polymers in Advanced Material Systems: Aerogels and Hybrid Materials.

**Recommended/Suggested Readings**

1. J. L. Fried, "Polymer Science and Technology", 3<sup>rd</sup> ed., 2014, Pearson Education. ISBN 978-0137039555
2. G. Odion, "Principles of Polymerization", 4<sup>th</sup> ed., 2007, Wiley USA. ISBN 978-8126513918.
3. A. Ravve, "Principles of Polymer Chemistry", 3<sup>rd</sup> ed., 2012, Springer-Verlog New York Inc. ISBN 978-1461422112
4. A. N, Wilkinson, A. J. Ryan, "Polymer Processing and Structure Development", New ed., 1999, Kluwer Academic Publishers. ISBN 978-0792357728
5. P. Ghosh, "Polymer Science and Technology: Plastics, Rubber, Blends and Composites", 3<sup>rd</sup> ed., McGraw Hill Education. ISBN 978-0070707047

**Course Outcomes**

1. Differentiate polymerization mechanisms (step-growth, chain-growth, and living polymerization) and analyze their role in synthesizing polymers with tailored properties.
2. Correlate polymer structure (molecular weight, crystallinity) with thermal, mechanical, and chemical behavior to predict material performance.
3. Apply characterization techniques (GPC, DMA, and spectroscopy) to assess molecular, rheological, and morphological properties of polymers.
4. Design polymer-based solutions for industries like biomedical engineering, sustainable packaging, and energy storage, emphasizing ethical and environmental considerations.

## Programme Elective - V

**Course Name: Medicinal Chemistry**

**Code: CHM-7216**

**Credits: 4**

### **Course Objectives**

This course aims to provide a comprehensive understanding of the principles and applications of medicinal chemistry, focusing on drug discovery, design, and development. Students will explore the physicochemical properties of drugs, mechanisms of drug action, pharmacokinetics, and pharmacodynamics. The course also covers modern drug design strategies, natural products, therapeutic agents, and emerging trends such as drug resistance, molecular diagnostics, and green chemistry. By the end, learners will be equipped to critically analyze drug development processes and apply this knowledge to real-world challenges in the pharmaceutical industry.

### **Block I: Fundamentals and Principles of Medicinal Chemistry**

#### **Unit 1: Introduction to Medicinal Chemistry**

Definition and Scope of Medicinal Chemistry, Drug Discovery and Development: Historical Perspectives and Modern Approaches, Classification of Drugs Based on Structure, Function and Pharmacological Activity, Physicochemical Properties Influencing Drug Action: Lipophilicity, Ionization and Solubility.

#### **Unit 2: Mechanisms of Drug Action**

Interaction of Drugs with Enzymes and Receptors, Agonists, Antagonists and Allosteric Modulators, Structure-Activity Relationships (SAR), Concept of Pharmacophores and Molecular Docking in Drug Design.

#### **Unit 3: Drug Metabolism**

Phases of Drug Metabolism: Oxidation, Reduction, Hydrolysis and Conjugation, Role of Cytochrome P450 Enzymes, Metabolic Activation and Inactivation of Drugs, Toxicological aspects of Drug Metabolism.

#### **Unit 4: Pharmacokinetics and Pharmacodynamics**

Absorption, Distribution, Metabolism and Excretion (ADME), Drug Bioavailability and Half-Life, Dose-Response Relationships and Therapeutic Index, Factors Affecting Drug Action and Response.

### **Block II: Drug Design and Development**

#### **Unit 5: Strategies in Drug Design**

Rational Drug Design: Structure-Based and Ligand-Based Approaches, Quantitative Structure-Activity Relationship (QSAR), Lead Identification and Optimization, Computer-Aided Drug Design (CADD).

#### **Unit 6: Prodrugs and Drug Delivery Systems**

Concept and Applications of Prodrugs, Targeted Drug Delivery: Liposomes, Nanoparticles and Hydrogels, Drug Release Mechanisms and Controlled Delivery Systems, Challenges in Drug Delivery Technologies.

#### **Unit 7: Combinatorial Chemistry and High-Throughput Screening**

Principles of Combinatorial Synthesis, Techniques for Library Generation and Screening, Applications of High-Throughput Screening in Drug Discovery, Automation and Robotics in Medicinal Chemistry Research.

#### **Unit 8: Natural Products in Drug Discovery**

Role of Natural Products as Lead Molecules, Sources of Bioactive Compounds: Plants, Microorganisms and Marine Organisms, Isolation and Characterization of Natural Products, Case

Studies of Natural Product-Derived Drugs.

### **Block III: Therapeutic Agents and Applications**

#### **Unit 9: Chemotherapeutic Agents**

Antibiotics: Penicillins, Cephalosporins and Tetracyclines, Antiviral Drugs: Mechanisms and Examples (E.G., Acyclovir, Oseltamivir), Anticancer Drugs: Alkylating Agents, Antimetabolites and Natural Products, Antifungal and Antiparasitic Drugs.

#### **Unit 10: Drugs for Cardiovascular and CNS Disorders**

Antihypertensives, Antiarrhythmics and Anticoagulants, Drugs for Neurodegenerative Diseases: Alzheimer's and Parkinson's, Antidepressants, Antipsychotics and Anxiolytics, Mechanisms of Drug Action for CNS-Related Disorders.

#### **Unit 11: Anti-inflammatory and Analgesic Agents**

Nonsteroidal Anti-Inflammatory Drugs (NSAIDs), Opioid and Non-Opioid Analgesics, Mechanisms of Action and Therapeutic Applications, Drugs for Rheumatoid Arthritis and Gout.

#### **Unit 12: Hormones and Endocrine Drugs**

Steroid and Non-Steroid Hormone Therapies, Drugs for Diabetes: Insulin and Oral Hypoglycemic Agents, Thyroid and Anti-Thyroid Drugs, Mechanisms and Therapeutic uses of Hormonal Drugs.

### **Block IV: Emerging Trends in Medicinal Chemistry**

#### **Unit 13: Drug Resistance and Remedial Measures**

Mechanisms of Drug Resistance in Bacteria, Viruses and Cancer Cells, Strategies to Combat Resistance: Combination Therapy and Drug Modification, Development of Novel Antibiotics and Antivirals, Case Studies of Resistance in Clinical Settings.

#### **Unit 14: Molecular Diagnostics and Biomarkers**

Role of Molecular Diagnostics in Drug Development, Biomarkers for Disease Diagnosis and Drug Response Prediction, Companion Diagnostics in Precision Medicine, Applications in Cancer, Infectious Diseases and Rare Disorders.

#### **Unit 15: Regulatory and Ethical Aspects in Medicinal Chemistry**

Overview of Drug Regulatory Authorities (FDA, EMA, CDSCO), Clinical Trials: Phases, Design, and Ethical Considerations, Intellectual Property Rights (IPR) and Patenting of Drugs, Ethical Issues in Drug Development and Marketing.

#### **Unit 16: Green Methods in Drug Development**

Principles of Green Chemistry in Medicinal Chemistry, Eco-Friendly Synthetic Methods, Role of Biocatalysis and Renewable Resources in Drug Synthesis, Case Studies of Sustainable Drug Development.

### **Books Recommended/Suggested Reading**

1. G. L. Patrick, "An Introduction to Medicinal Chemistry", 3<sup>rd</sup> ed., 2005, Oxford University Press. ISBN 978-0199275007
2. V. F. Roche, S. W. Zito, T. M. Lemke, D. A. Williams, "Foye's Principles of Medicinal Chemistry". 8<sup>th</sup> ed., 2019, Wolters Kluwer Publishers. ISBN 978-1975139032
3. C. G. Wermuth, "The Practice of Medicinal Chemistry", Standard ed., 2009, Elsevier Science. ISBN 978-8131219614
4. R. L. Brunton, B. C. Knollmann, "Godman and Gilman's The Pharmacological Basis of Therapeutics", 14<sup>th</sup> ed., 2023, McGraw Hill Publication. ISBN 978-1265016982
5. R. G. Hill, D. B. Richards, "Drug Discovery and Development: Technology in Transition", 3<sup>rd</sup> ed. 2021, Elsevier Health Sciences. ISBN 978-0702078040

**Course Outcomes**

On successful completion of this course, students shall be able to

1. Explain the fundamental principles of medicinal chemistry, including drug classification, physicochemical properties, and mechanisms of drug action.
2. Analyze the processes of drug metabolism, pharmacokinetics, and pharmacodynamics, and their impact on drug efficacy and safety. Apply modern drug design strategies, including structure-based and ligand-based approaches, to identify and optimize lead compounds.
3. Evaluate the role of natural products, combinatorial chemistry, and high-throughput screening in drug discovery and development.
4. Discuss emerging trends such as drug resistance, molecular diagnostics, and green chemistry, and their implications for sustainable drug development.

**Course Objectives**

This course aims to introduce students to the principles and practices of green chemistry through a series of laboratory experiments. By performing a minimum of six experiments, including three synthetic preparations, students will explore environmentally friendly methods and sustainable practices in chemical synthesis and extraction. The focus is on using green solvents, alternative energy sources (such as microwaves and sunlight), and innovative techniques like ultrasound and supercritical CO<sub>2</sub> extraction. The course emphasizes the importance of atom economy, biocatalysis, and the conversion of waste into valuable products, fostering a deeper understanding of the environmental and safety benefits of green chemistry.

**Green Chemistry (Minimum six experiments will be performed including 3 preparations)**

1. Synthesis of Aspirin Using Green Solvents.
2. Microwave-Assisted Synthesis of Benzimidazole.
3. Photochemical Synthesis of Benzoin Using Sunlight.
4. Ultrasound-Assisted Synthesis of Chalcones
5. Extraction of Natural Products Using Supercritical CO<sub>2</sub>.
6. Solvent-Free Aldol Condensation.
7. Evaluation of Atom Economy in a Reaction
8. Baeyer-Villiger Oxidation Using Biocatalysis.
9. To convert agricultural waste into bioethanol through fermentation.
10. To evaluate the safety and environmental impact of a green vs. traditional synthesis process.

**Books Recommended/Suggested Readings**

1. M. Lancaster, "Green Chemistry: An Introductory Text", 2<sup>nd</sup> ed., 2010, Royal Society of Chemistry. ISBN 978-1847558732
2. P. T. Anastas, J. C. Warner, "Green Chemistry: Theory and Practice", Reprint, 2005, Oxford University Press, UK. ISBN 978-0198506980
3. R. A. Sheldon, I. Arends, U. Hanefeld, "Green Chemistry and Catalysis", 2006, Wiley-VCH Verlag GmbH. ISBN 978-3527611003
4. S. K. Sharma, A. Mudhoo, "Green Chemistry for Environmental Sustainability", 2019, CRC Press. ISBN 978-1032297903

**Course Outcomes**

1. Students will demonstrate the ability to apply green chemistry principles in the synthesis and extraction of chemical compounds, utilizing environmentally friendly techniques and solvents.
2. Students will develop the skills to critically evaluate the environmental and safety impacts of green versus traditional chemical processes, with an emphasis on atom economy, waste reduction, and sustainability.
3. Students will gain hands-on experience with innovative green chemistry techniques, such as microwave-assisted synthesis, photochemical reactions using sunlight, and the use of supercritical CO<sub>2</sub> for natural product extraction, enhancing their practical laboratory skills and knowledge of sustainable practices.



**Course Objectives**

The objective of this M.Sc. Chemistry course is to provide students with hands-on experience in various specialized areas of chemistry through practical experiments. By conducting experiments in Supramolecular Chemistry, Materials Chemistry, Chemistry of Natural Products, Polymer Chemistry, and Medicinal Chemistry, students will gain a deeper understanding of synthesis, characterization, and analysis techniques. These practical skills will complement their theoretical knowledge and prepare them for advanced research and professional applications in the chemical sciences.

**(Students need to perform the experiments of their respective programme elective courses only)**

**Supramolecular Chemistry (three experiments will be performed)**

1. Synthesis of a crown ether and test of its binding affinity toward alkali metal ions.
2. Study a model reaction (e.g., hydrolysis of esters) catalyzed by a supramolecular host.
3. Prepare cyclodextrin derivatives and study drug encapsulation using NMR spectroscopy.
4. Prepare and analyze host-guest complexes involving fullerenes using spectroscopy.
5. Synthesis a metal-organic framework and study its gas adsorption properties.

**Materials Chemistry (three experiments will be performed)**

1. Synthesis of Zinc Oxide Nanoparticles via Sol-Gel Process and Characterization thereof.
2. Solid-State Synthesis of BaTiO<sub>3</sub> and Characterization Using Powder X-ray Diffraction (PXRD).
3. Preparation of Polyaniline as a Conducting Polymer and Measurement of Its Electrical Conductivity.
4. Synthesis of a Biodegradable Polymer (e.g., Polylactic Acid) and Study of Its Thermal Properties Using Differential Scanning Calorimetry (DSC).
5. Synthesis of a Semiconductor (ZnS or CdS) via Solvothermal Method and Study of Its Band Gap Using UV-Vis Spectroscopy.

**Chemistry of Natural Products (three experiments will be performed)**

1. Extraction of primary and secondary metabolites from a plant source (e.g., alkaloids, terpenoids, flavonoids).
2. Extraction of lipids from seeds and their characterization by iodine value or saponification value.
3. Quantitative Estimation of Vitamin C in Citrus Fruits.
4. Extraction and purification of streptomycin.
5. Isolation of cholesterol from egg yolk and separation using TLC.

**Polymer Chemistry (three experiments will be performed)**

1. Synthesis of Polymethyl Methacrylate (PMMA) by Radical Polymerization.
2. Living Polymerization of Methyl Methacrylate (MMA) using RAFT Technique.
3. Synthesis of Polystyrene by Suspension Polymerization and examination of its particle size distribution.
4. To determine the glass transition temperature (T<sub>g</sub>) and melting point (T<sub>m</sub>) of a polymer.
5. To determine the molecular weight and polydispersity index of a given polymer.

**Medicinal Chemistry (three experiments will be performed)**

1. Analysis of Drug Solubility and its  $pK_a$  by potentiometric titration.
2. Determination of Partition Coefficient of a Drug Molecule.
3. Kinetic Study of Drug Release from a Formulation.
4. Green Synthesis of a Pharmaceutical Compound.
5. Study of the Interaction between NSAIDs and Proteins by Spectrophotometry.

#### **Books Recommended/Suggested Readings**

1. J. W. Steed, J. L. Atwood, "Supramolecular Chemistry", 3<sup>rd</sup> ed., 2022, Wiley, USA. ISBN 978-1119582519.
2. J. B. Baruah, "Principles and Application of Supramolecular Catalysis", 1<sup>st</sup> ed., 2019, CRC Press Ltd. ISBN 978-0367111649
3. W. D. Callister, D. G. Rethwisch, "Materials Science and Engineering: An Introduction", 10<sup>th</sup> ed., 2020, Wiley USA. ISBN 978-1119721772
4. W. D. Kingery, H. K. Bowen, Uhlman, "Introduction to Ceramics", 2<sup>nd</sup> ed., 2012, Wiley India Pvt. Ltd. ISBN 978-8126539994
5. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Bantrophe, J. b. Harborne, "Natural Products: Their Chemistry and Biological Significance", 1<sup>st</sup> ed., 1994, Longman Group UK Limited. ISBN 978-0582060098
6. P. M. Dewick, "Medicinal Natural Products: A Biosynthetic Approach", 3<sup>rd</sup> ed., 2009, John Wiley & Sons Inc. ISBN 978-0470741689
7. J. L. Fried, "Polymer Science and Technology", 3<sup>rd</sup> ed., 2014, Pearson Education. ISBN 978-0137039555
8. G. Odion, "Principles of Polymerization", 4<sup>th</sup> ed., 2007, Wiley USA. ISBN 978-8126513918
9. G. L. Patrick, "An Introduction to Medicinal Chemistry", 3<sup>rd</sup> ed., 2005, Oxford University Press. ISBN 978-0199275007
10. V. F. Roche, S. W. Zito, T. M. Lemke, D. A. Williams, "Foye's Principles of Medicinal Chemistry". 8<sup>th</sup> ed., 2019, Wolters Kluwer Publishers. ISBN 978-1975139032

#### **Course Outcomes**

1. Students will acquire hands-on experience in synthesizing and characterizing chemical compounds, using a variety of advanced laboratory techniques.
2. The practical exercises will enable students to apply their theoretical understanding of chemical principles to real-world experimental scenarios, enhancing their problem-solving and analytical skills.
3. By completing these experiments, students will be well-prepared for further research in academia or professional roles in the chemical industry, equipped with practical skills and in-depth knowledge of specialized areas in chemistry.

**Course Name: Project**

**Code: CHM-7291**

**Credits: 6**

**Course Objectives**

The objective of the course is to work with students to identify mathematical problem. The course also focuses to find out probable solution of that mathematical problem.

**Syllabus**

Every student shall, in the Fourth (final) Semester, submit a Dissertation reporting the results of original research on a topic assigned at the beginning of the semester by the concerned research guide (faculty member) in consultation with the student, in his/her area(s) of special interest. The research guide shall be chosen by the student according to his/her interest and the faculty member's area of expertise. No faculty member shall guide more than five students.

The topic of the Dissertation shall be approved by the Head of the Department. For this purpose, the candidate shall submit to the Head an application stating the topic for the dissertation along with a synopsis within three weeks of the commencement of classes of the Fourth Semester. Once approved, the topic of dissertation shall not be altered without a fresh proposal from the student accompanied by a written request stating the reason for change. No such request shall be entertained after five weeks of the commencement of classes of the Semester in question.

**Course Outcomes**

On successful completion of this course, students shall be able to

1. Identify and Define appropriate research problems.
2. Explain appropriate research approaches for solving problems.
3. Apply various tools and techniques to complete research.
4. Analyse research report and make robust conclusion.

**Course Objectives**

This course aims to provide a comprehensive understanding of environmental chemistry, focusing on the fundamental principles governing natural ecosystems and human-induced environmental changes. Students will explore the chemistry of air, water, and soil, along with pollution control techniques, environmental laws, and emerging trends like green chemistry and renewable energy. The course emphasizes the application of chemical knowledge to address real-world environmental challenges and promote sustainable practices.

**Block I: Fundamentals of Environmental Chemistry**

**Unit 1: Introduction to the Environment**

Definition, scope, and importance of the environment, Components of the environment: Lithosphere, Hydrosphere, Atmosphere, and Biosphere, Interdependence of physical, biological, and social components, Structure and function of ecosystems, Types of ecosystems: terrestrial, aquatic, and artificial, Energy flow in ecosystems: Food chains, food webs, and ecological pyramids

**Unit 2: Chemistry of the Atmosphere**

Composition and Structure of the Atmosphere, Chemical and Photochemical Reactions in the Atmosphere, Ozone Chemistry and Depletion, Greenhouse Gases and Global Warming.

**Unit 3: Chemistry of Water**

Properties of Water: Physical and Chemical Characteristics, Water Pollution: Sources and Types (Organic, Inorganic, Thermal, Radioactive etc.), Eutrophication and Algal Blooms, Water Quality Parameters and Standards.

**Unit 4: Soil Chemistry**

Composition of Soil and Soil Formation, Soil Pollutants: Sources and Impacts, Soil pH, Cation Exchange Capacity and Nutrient Cycles, Soil Remediation Techniques.

**Unit 5: Biogeochemical Cycles**

Carbon, Nitrogen, Phosphorus and Sulfur Cycles, Human Impact on Biogeochemical Cycles, Interdependence of Cycles in Environmental Processes, Role of Microbes in Biogeochemical Transformations.

**Block II: Environmental Pollution and Control**

**Unit 6: Air Pollution**

Sources and Types of Air Pollutants, Acid Rain and Smog: Formation and Effects, Measurement and Control of Air Pollution, Indoor Air Pollution and its Mitigation.

**Unit 7: Water Pollution and Treatment**

Industrial and Domestic Water Pollutants, Wastewater Treatment Processes: Primary, Secondary and Tertiary Treatments, Advanced Oxidation Processes for Water Treatment, Membrane Technologies in Water Purification.

**Unit 8: Solid Waste Management**

Classification of Solid Waste: Hazardous and Non-Hazardous, Waste Treatment Methods: Composting, Incineration and Landfill Management, Recycling and Resource Recovery, Management of Electronic Waste and Biomedical Waste.

**Unit 9: Noise and Radiation Pollution**

Sources and Measurement of Noise Pollution, Impacts of Noise Pollution on Human Health and Environment, Sources of Radioactive Pollution and Effects on Living Organisms, Methods for Noise

and Radiation Pollution Control.

### **Block III: Environmental Laws, Policies, and Legislation**

#### **Unit 10: International Environmental Agreements**

Montreal Protocol, Kyoto Protocol and Paris Agreement, Stockholm and Basel Conventions, Role of the United Nations in Environmental Protection, Transboundary Pollution and Global Initiatives.

#### **Unit 11: Environmental Policies and Laws in India**

Environment Protection Act, Water Act and Air Act, Forest Conservation Act and Wildlife Protection Act, National Green Tribunal: Structure and Role, Policies on Hazardous Waste and E-Waste Management.

#### **Unit 12: Environmental Impact Assessment (EIA)**

Purpose and Process of EIA, Screening, Scoping and Public Consultation, Environmental Management Plans (EMP), Case Studies of Successful EIA Implementation.

#### **Unit 13: Climate Change and Sustainability Policies**

National Action Plan on Climate Change (NAPCC), Renewable Energy Policies In India, Sustainable Development Goals (SDGs), Role of Industries in Achieving Environmental Sustainability.

### **Block IV: Emerging Trends in Environmental Chemistry**

#### **Unit 14: Green Chemistry and Sustainable Practices**

Principles of Green Chemistry, Green Solvents and Renewable Feedstocks, Catalysis and Atom Economy in Sustainable Processes, Industrial Applications of Green Chemistry.

#### **Unit 15: Environmental Analytical Techniques**

Sampling and Sample Preparation, Spectroscopic and Chromatographic Techniques for Pollutant Analysis, Electrochemical Methods for Environmental Monitoring, Remote Sensing and GIS in Environmental Studies.

#### **Unit 16: Emerging Pollutants and Their Management**

Persistent Organic Pollutants (Pops), Microplastics and Nanomaterials in the Environment, Pharmaceuticals and Personal Care Products as Pollutants, Strategies for Managing Emerging Pollutants.

#### **Unit 17: Renewable Energy and Environmental Chemistry**

Chemistry of Solar Cells and Photovoltaics, Biofuels and Hydrogen Energy, Waste-to-Energy Technologies, Role of Chemistry in Carbon Capture and Storage.

### **Books Recommended/Suggested Reading**

1. S. E. Manahan, "Environmental Chemistry", 11<sup>th</sup> ed., 2022, CRC Press. ISBN 978-0367558871
2. G. M. Masters, W. P. Ela, "Introduction to Environmental Engineering and Science", 3<sup>rd</sup> ed., 2015, Pearson Education India. ISBN 978-9332549760
3. S. Divan, A. Rosencranz, "Environmental Law and Policy in India", 3<sup>rd</sup> ed., 2023, Oxford University Press. ISBN 978-0192871831
4. A. Boyle, C. Redgwell, "International Law and the Environment" 4<sup>th</sup> ed., 2021, Oxford University Press. ISBN 978-0199594016
5. P. T. Anastas, J. C. Warner, "Green Chemistry: Theory and Practice", Reprint, 2005, Oxford University Press, UK. ISBN 978-0198506980
6. S. K. Sharma, A. Mudhoo, "Green Chemistry for Environmental Sustainability", 2019, CRC Press. ISBN 978-1032297903

### **Course Outcomes**

On successful of this course, students will be able to

1. Explain the structure and function of ecosystems, biogeochemical cycles, and the interdependence of environmental components.
2. Analyze the sources, impacts, and control measures of air, water, soil, and noise pollution.
3. Evaluate the role of international and national environmental policies, laws, and impact assessments in addressing environmental issues.
4. Apply principles of green chemistry and sustainable practices to mitigate environmental pollution and promote resource efficiency.
5. Utilize analytical techniques and emerging technologies to monitor and manage environmental pollutants effectively.

**Course Objectives**

The primary objective of this course is to provide students with hands-on experience in analyzing environmental pollutants using various analytical techniques. Through a series of experiments, students will learn to measure and interpret data related to air, water, and soil quality, employ green chemistry principles in synthesizing sustainable products, and understand the application of advanced instrumental methods like Atomic Absorption Spectroscopy (AAS) and UV-Visible Spectroscopy in environmental analysis. These practical skills are essential for addressing real-world environmental challenges and contributing to sustainable development.

**(At least six experiments will be performed)**

1. Analysis of gaseous pollutants like SO<sub>2</sub> and NO<sub>2</sub> using spectrophotometry.
2. Determination of pH, moisture content, and organic matter in soil.
3. Measurement of pH, turbidity, conductivity, and total dissolved solids (TDS) of the given water sample.
4. Analysis of heavy metal content in soil using Atomic Absorption Spectroscopy (AAS).
5. Synthesis of biodiesel from vegetable oils using green chemistry principles.
6. Titrimetric analysis of chloride ions using the Mohr or Volhard method.
7. Analysis of nitrate content in water using UV-Visible Spectroscopy.
8. Determination of lead or cadmium in water using AAS.
9. Measurement of ambient ozone levels using the iodometric method.
10. Analysis of NO<sub>x</sub> in air samples using spectrophotometric methods.
11. Demonstration of coagulation and flocculation processes in water purification.
12. Study of the efficiency of activated carbon in removing organic dyes or heavy metals from water.
13. Synthesis and applications of nanomaterials like ZnO or TiO<sub>2</sub> for pollutant remediation (minimum 1).
14. Identification of Pesticides in Pesticide Residues.
15. Determination of Available Nitrogen in a Soil sample.
16. Determination of Available Sulphur in a Soil Sample.
17. Determination of Extractable Manganese and Iron in a Soil Sample

**Recommended Books/Suggested Readings**

1. S. E. Manahan, "Environmental Chemistry", 11<sup>th</sup> ed., 2022, CRC Press. ISBN 978-0367558871
2. G. M. Masters, W. P. Ela, "Introduction to Environmental Engineering and Science", 3<sup>rd</sup> ed., 2015, Pearson Education India. ISBN 978-9332549760
3. F. M. Dunnivant, J. W. Ginsbach, "Essential Methods of Instrumental Analysis", 1<sup>st</sup> ed., 2024, John Wiley & Sons Inc. USA. ISBN 978-1394226719
4. D. A. Skoog, F. J. Holler, S. R. Crouch "Principles of Instrumental Analysis", 7<sup>th</sup> ed., 2018, Cengage Learning. ISBN 978-9353506193

**Course Outcomes**

1. Students will gain practical experience in using various analytical instruments and methods to measure environmental pollutants in air, water, and soil, enhancing their technical skills in environmental monitoring and analysis.
2. Through experiments such as the synthesis of biodiesel and nanomaterials, students will learn to apply green chemistry principles, fostering a sustainable approach to chemical processes and

pollutant remediation.

3. By engaging in real-world environmental analysis and interpreting experimental data, students will develop critical thinking and problem-solving skills, preparing them to address complex environmental issues and contribute to research and development in environmental science.

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### **Faculty and Support Staff**

The University has identified the requisite faculty and support staff as mandated by UGC and formally they shall be allocated the required positions from amongst the existing faculty exclusively for ODL mode or fresh appointments as required so, shall be initiated for which Letter of Intent have been issued to the prospective faculty and staff. The course material prepared by this university will be on par with any open university/Distance education centre in the country.

**List of Faculty associated with MSc- Chemistry programme is as follows:-**

| <b>S. No.</b> | <b>Name of Faculty</b> | <b>Designation</b>  | <b>Nature of Appointment</b> | <b>Qualification</b> | <b>Subject</b> |
|---------------|------------------------|---------------------|------------------------------|----------------------|----------------|
| 1             | Prof. Ravi Kant        | Professor           | Full Time                    | Ph.D.                | Chemistry      |
| 2             | Dr. Monika Singh       | Associate Professor | Full Time                    | Ph.D.                | Chemistry      |

### **Delivery Mechanism**

**The mode of programme delivery will be ODL.**

The ODL of MU provides flexible learning opportunities by overcoming the separation of teachers and learners to deliver teaching and learning experiences. The University also follows a modern ICT (Information & Communication Technology) enabled approach for instruction. The methodology of instruction in ODL of MU is different from that of the conventional/regular programmes. Our ODL system is more learner-oriented and the learner is an active participant in the teaching-learning process. ODL of MU academic delivery system comprises:

#### **A. Print Material**

The printed material of the programme supplied to the students will be unit wise for every course.

#### **B. Counselling Sessions**

Normally, counselling sessions are held as per a schedule drawn beforehand by the Subject Coordinator. There will be 6 counselling/ contact classes for 4 credit courses will be held on the campus on Saturday and on Sunday of 2 hour duration for each course in face to face mode (In case of 2 credit course contact hours are required 6 hours and in case of 6 credit course contact hours required 18 hours ). Contact classes will be held in the campus on Saturdays and on Sundays.

#### **C. Medium of Instruction**

Medium of Course Instruction: English

Medium of Examination: English

#### **Student Support Systems:**

Universities Study Centres or Learner Support Centre shall be headed by a coordinator, not below the rank of Assistant professor and shall be augmented with academic and non-academic staff depending on the learner.

The university has made appropriate arrangements for various support services including counseling schedule and resource-oriented services evaluation methods and dates both online and offline modes for easy and smooth services to the students of distance mode.

At present the university have only one study centre on the campus. The institution is not promoting any study centers outside the campus. All student support services will be provided to the student through a single window method/mode onsite and online.

**Procedure for Admissions, Curriculum, Transaction and Evaluation Admission Process**

Admission to the M.Sc. (Chemistry) Programme will be done on the basis of screening of candidate’s eligibility on first come first serve basis. The University will follow the reservation policy as per norms of the Government. Admission shall not be a right to the students and MU, CDOE shall retain the right to cancel any admission at any point of time if any irregularity is found in the admission process, eligibility etc.

**Maximum Duration**

A. The maximum duration of the M.Sc. (Chemistry) Programme is four years. Thereafter, students seeking completion of the left-over course(s) will be required to seek fresh admission.

B. The student can complete his programme within a period of 4 years failing which he/she shall seek fresh admission to complete the programme.

**Eligibility**

Science (PCM/PCMB) Graduate from a recognised University is eligible for admission into M.Sc. (Chemistry) programme.

**Fee Structure**

| Name of the Programme         | Degree | Duration     | Year | Tuition Fee/Year | Exam Fee/Year | Total (in Rs.) |
|-------------------------------|--------|--------------|------|------------------|---------------|----------------|
| Master of Science (Chemistry) | PG     | 2 to 4 Years | 1    | 15000            | 2000          | 17000          |
|                               |        |              | 2    | 13500            | 2000          | 15500          |
| <b>Total</b>                  |        |              |      |                  |               | <b>32500</b>   |

### Activity Schedule

| S. No. | Name of the Activity                             | Tentative months schedule (specify months) during year |     |      |     |
|--------|--|--|-----|------|-----|
|        |  | From   | To  | From | To  |
| 1      | Admission  | Jul  | Sep | Jan  | Mar |
| 2      | Assignment submission (if any)                   | Sep  | Oct | Mar  | Apr |
| 3      | Evaluation of Assignment                         | Oct  | Nov | Apr  | May |
| 4      | Examination                                      | Dec  |     | Jun  |     |
| 5      | Declaration of Result                            | Jan  |     | Jul  |     |
| 6      | Re-registration                                  | Jul  |     | Jan  |     |
| 7      | Distribution of SLM                              | Jul  | Sep | Jan  | Mar |
| 8      | Contact Programmes (counseling, Practicals.etc.) | Sep  | Nov | Mar  | May |

### Credit System

MU, CDOE proposes to follow the 'Credit System' for most of its programmes. Each credit amounts to 30 hours of study comprising all learning activities. Thus, an 8 credit course requires 240 hours, 6 credit course requires 180 hours, 4 credit course requires 120 hours and 2 credit course requires 60 hours of study. This helps the student to understand the academic effort to complete a course. Completion of an academic programme requires successful clearing of both, the assignments and the term-end examination of each course in a programme.

| Duration of programme | Credits | Name of programme | Level of programme |
|-----------------------|---------|-------------------|--------------------|
| 2 to 4 Yrs.           | 80      | M.Sc. (Chemistry) | Master's Degree    |

### Assignments

Distance Education learners have to depend much on self study. In order to ascertain the writing skill and level of comprehension of the learner, assignment work is compulsory for all learners. Each assignment shall consist of a number of questions, case studies and practical related tasks. The Assignment Question Papers will be uploaded to the website within a scheduled time and the learners shall be required to respond them within a specified period of time. The response of the learner is examined by a faculty member.

**Evaluation:** The evaluation system of the programme is based on two components:

**Continuous Evaluation in the form of assignments (weightage 30%):** This Component carries a weightage of 30%. There will be at least one graded assignment and test per course. These assignments are to be submitted to the Coordinator of the CDOE/Study Centre to which the student is assigned or attached with.

**Term-end examination (weightage 70%):** This will be held twice every year in the months of June and December. The students are at liberty to appear in any of the examinations conducted by the University during the year. A student will be allowed to appear in the Term-End Examination only after she/he has registered for that course and submitted the assignment. For appearing in the Examination, every student has to submit an Examination form through online ([www.mangalayatan.in](http://www.mangalayatan.in))/ or offline before the due dates as given in the schedule of operations. If a student misses any term-end examination of a course for any reason, s/he may appear for any of them or all the courses subject to the maximum of 8 courses in the subsequent term-end examinations. This facility will be available until a student secures the minimum pass grade in the courses but up to a maximum period of four semesters, since the date of registration of the course is valid for four semesters. Beyond this period s/he may continue for another four semesters by getting Re-registration by paying fee again. In that case, the score of qualified assignments and/or term-end examination will be retained and the student will be required to complete the left out requirements of such re-registered courses. Minimum requirement for passing a course will be 40% marks.

### **Laboratory Support and Library Resources**

The library of Mangalayatan University aims to empower the teaching mission and intellectual culture of the community through availability through an organized collection of information as well as instruction in its access, relevance and evaluation. The University Library enriches advance learning and discovery by providing access to a broad array of resources for education, research and creative work to ensure the rich interchange of ideas in the pursuit of knowledge.

The Centre of Distance Education of Mangalayatan University has initiated the process of setting up a dedicated Library for ODL programme and acquiring printed books and e-books for this purpose. The required International and National subject journals are also provided. We have a full functioning community radio service onboard (90.4 FM). We already have annual journal subscriptions and the capacity can be enlarged at later stages as the University lines up with more online journals.

The collection of the Library is rich and diverse especially in terms of the breadth and depth of coverage. Collection encompasses subjects in Management, Commerce, Information Technology, Computer Applications, and other allied areas. This collection further includes Books, Research Journals, Project Reports/Dissertations and online Journals.

The Chemistry laboratory is well equipped with chemicals, reagents as well as instruments which are necessary for practical analysis.

The University has well equipped Computer Laboratories, Lecture Capturing Systems, Audio Video facilities, ICT enabled class rooms, Wi-Fi facilities etc.

### **Cost estimate of the programme and the provisions**

Initial expenses have been done by the University in terms of provision of infrastructure, manpower, printing of Self Study Material etc. The University intends to allocate expenses out of the total fee collection as per following details:

- a) SLM Development and Distribution: 20%

- b) Postal and ICT Expenses: 10%
- c) Salary and other Administrative expenses: 60%
- d) Future Research development reserve: 10%

Once programmes are operational, the programme budget from fee receipts will be planned as per the guidelines of University Grants Commission.

### **Quality Assurance**

The University has established the Centre for Internal Quality Assurance (CIQA) in the University campus. The CIQA will monitor and maintain the quality of the ODL programmes. It has the following objectives in making the compliances of quality implementations.

### **Objectives**

The objective of Centre for Internal Quality Assurance is to develop and put in place a comprehensive and dynamic internal quality assurance system to ensure that programmes of higher education in the Open and Distance Learning mode and Online mode being implemented by the Higher Educational Institution are of acceptable quality and further improved on continuous basis.

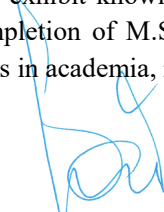
### **Functions of CIQA**

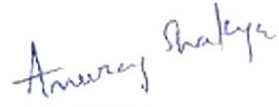
The functions of Centre for Internal Quality Assurance would be following:

- 1) To maintain quality in the services provided to the learners.
- 2) To undertake self-evaluative and reflective exercises for continual quality improvement in all the systems and processes of the Higher Educational Institution.
- 3) To contribute in the identification of the key areas in which Higher Educational Institution should maintain quality.
- 4) To devise mechanism to ensure that the quality of Open and Distance Learning programmes and Online programmes matches with the quality of relevant programmes in conventional mode.
- 5) To devise mechanisms for interaction with and obtaining feedback from all stakeholders namely, learners, teachers, staff, parents, society, employers, and Government for quality improvement.
- 6) To suggest measures to the authorities of Higher Educational Institution for qualitative improvement.
- 7) To facilitate the implementation of its recommendations through periodic reviews.
- 8) To organize workshops/seminars/symposium on quality related themes, ensure participation of all stakeholders, and disseminate the reports of such activities among all the stakeholders in Higher Educational Institution.
- 9) To develop and collate best practices in all areas leading to quality enhancement in services to the learners and disseminate the same all concerned in Higher Educational Institution.

- 10) To collect, collate and disseminate accurate, complete and reliable statistics about the quality of the programme(s).
- 11) To ensure that Programme Project Report for each programme is according to the norms and guidelines prescribed by the Commission and wherever necessary by the appropriate regulatory authority having control over the programme;
- 12) To put in place a mechanism to ensure the proper implementation of Programme Project Reports.
- 13) To maintain a record of Annual Plans and Annual Reports of Higher Educational Institution, review them periodically and generate actionable reports.
- 14) To provide inputs to the Higher Educational Institution for restructuring of programmes in order to make them relevant to the job market.
- 15) To facilitate system based research on ways of creating learner centric environment and to bring about qualitative change in the entire system.
- 16) To act as a nodal coordinating unit for seeking assessment and accreditation from a designated body for accreditation such as NAAC etc.
- 17) To adopt measures to ensure internalization and institutionalization of quality enhancement practices through periodic accreditation and audit.
- 18) To coordinate between Higher Educational Institution and the Commission for various qualities related initiatives or guidelines.
- 19) To obtain information from other Higher Educational Institutions on various quality benchmarks or parameters and best practices.
- 20) To record activities undertaken on quality assurance in the form of an annual report of Centre for Internal Quality Assurance.
- 21) It will be mandatory for Centre for Internal Quality Assurance to submit Annual Reports to the Statutory Authorities or Bodies of the Higher Educational Institution about its activities at the end of each academic session. A copy of report in the format as specified by the Commission, duly approved by the statutory authorities of the Higher Educational Institution shall be submitted annually to the Commission.

After enrolling in M.Sc. (Chemistry) programme of Mangalayatan University in ODL mode, student will exhibit knowledge, skill and general competence with scientific aptitude and innovation. After completion of M.Sc. (Chemistry) programme, student will pursue further studies in Chemistry for roles in academia, research, industry, laboratory, technology and government.

  
Registrar  
Mangalayatan University  
Beswan, Aligarh

  
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Centre for Distance and Online Education  
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