



**MASTER OF SCIENCE - CHEMISTRY
CURRICULUM AND SYLLABI**

**Learning Outcome based Curriculum Framework
(Effective from Academic year 2022)**

**Shri Ramasamy Memorial University Sikkim
5th Mile, Tadong, Gangtok, Sikkim 737102**

| Department Vision Statement | |
|------------------------------|--|
| Statement 1 | To create scholars with clear understanding of concepts of chemistry capable of pioneering discoveries and advancements in chemical research. |
| Statement 2 | To ignite learners' mind with problem-solving, critical thinking, and analytical reasoning skills with practical applications in diverse areas of Chemistry. |
| Statement 3 | To further prepare learners for World-class education, as well as to work independently in research or other industry settings and to generate nation-wide sustainable innovative solutions. |
| Department Mission Statement | |
| Statement 1 | To provide a thorough understanding of the concepts and principles of different domains of Chemistry. |
| Statement 2 | To arm the learners with skills to apply the theoretical concepts through basic and advanced experimental techniques. |
| Statement 3 | To empower learners to be internationally relevant, technologically proficient, and creative in order to generate professional human resources. |
| Statement 4 | To create a solid basis for higher education and professional learning while enabling them to find employment in a variety of research, academic, and industrial domains. |
| Statement 5 | To foster a scientific mind-set in society, teach learners uphold professional ethics, and use their understanding of chemistry to contribute to the environmental and sustainable advancement of society. |
| Program Objective (PO) | |
| PO - 1 | To develop the understanding of advanced topics on various areas of chemistry. |
| PO - 2 | To provide learners with an opportunity to conduct experiments using advanced analytical tools. |
| PO - 3 | To facilitate learners with the creative ideas in solving various chemical problems using the knowledge of various areas of chemistry and thus expediting their employability in industry and academia. |
| PO - 4 | To equip learners with effective written and oral communication skills and enable them to share their scientific findings and ideas to diverse stakeholders. |
| PO - 5 | To impart learners' a sense of professional ethics and responsibilities towards the sustainable society. |

PROGRAMME STRUCTURE

The Master of Science in Chemistry is a two-year course divided into four semesters. A student is required to earn 84 credits for the award of MSc degree.

| Year | Semester | |
|-------------|-----------------|-------------|
| First Year | Semester I | Semester II |
| Second Year | Semester III | Semester IV |

Each credit = 15 hours lecture. A student has to dedicate 1hour/week for 1 credit theory/tutorial course and 2 hours/week for 1 credit practical course.

Abbreviation

| | | | |
|------------|----------------------------|------------|------------------------------|
| L | No. of Lecture hours | T | No. of Tutorial hours |
| P | No. of Practical hours | C | No. of Credit hours |
| CT | Core Theory | DSE | Discipline Specific Elective |
| CP | Core Practical | OE | Open Elective |
| AEC | Ability Enhancement Course | P | Project |
| SEM | Semester | | |

MSc Curriculum

| SEM | Course Category | Course Name | Course Code | L | T | P | C |
|------------------------------|-----------------|---|-------------|----|---|---|---|
| I | CT | Mechanistic Aspects of Organic Chemistry | MCH2211 | 4 | 0 | 0 | 4 |
| | CT | Principles of Inorganic Chemistry | MCH2212 | 4 | 0 | 0 | 4 |
| | CT | Thermodynamics and kinetics | MCH2213 | 4 | 0 | 0 | 4 |
| | AEC | Mathematics for chemist | MCA2214 | 2 | 0 | 0 | 2 |
| | CP | Organic Qualitative Analysis | MCH2215 | 0 | 0 | 4 | 2 |
| | CP | Estimation of metals present in alloy/mixture | MCH2216 | 0 | 0 | 4 | 2 |
| | CP | Laboratory on kinetics, polymer and phase equilibria | MCH2217 | 0 | 0 | 4 | 2 |
| Total Credits in Semester I | | | | 20 | | | |
| | | | | | | | |
| II | CT | Synthetic Organic Chemistry | MCH2221 | 4 | 0 | 0 | 4 |
| | CT | Applied Inorganic Chemistry | MCH2222 | 4 | 0 | 0 | 4 |
| | CT | Principles, Theory and Applications of Spectroscopy | MCH2223 | 4 | 0 | 0 | 4 |
| | CT | Quantum Chemistry and Solid State chemistry | MCH2224 | 4 | 0 | 0 | 4 |
| | CP | Organic Synthesis (multistep) and Spectral Analysis | MCH2225 | 0 | 0 | 4 | 2 |
| | CP | Synthesis and Characterization of inorganic compounds | MCH2226 | 0 | 0 | 4 | 2 |
| | CP | Laboratory on Electrochemistry and Spectroscopy | MCH2227 | 0 | 0 | 4 | 2 |
| Total Credits in Semester II | | | | 22 | | | |
| | | | | | | | |
| III | CT | Implications of Organic Chemistry | MCH2231 | 4 | 0 | 0 | 4 |
| | CT | Chemistry of <i>d</i> and <i>f</i> block elements | MCH2232 | 4 | 0 | 0 | 4 |

| | | | | | | | | |
|--------------------------------|------------------------------------|---|---|---------|---|----|----|---|
| | CT | Fundamentals and applications of Electrochemistry | | MCH2233 | 3 | 0 | 0 | 3 |
| | CT | Analytical Chemistry | | MCH2234 | 3 | 0 | 0 | 3 |
| | DSE | Discipline Specific Elective I | Theoretical and Physical aspects of Organic Reactions | MCH2235 | 4 | 0 | 0 | 4 |
| | | | Supramolecular chemistry and modern crystal engineering | MCH2236 | | | | |
| | | | Computational Chemistry | MCH2237 | | | | |
| CP | Computational Chemistry Laboratory | | MCH2238 | 0 | 0 | 4 | 2 | |
| P | Project I | | MCH2239 | 0 | 0 | 4 | 2 | |
| Total Credits in Semester III | | | | | | 22 | | |
| | | | | | | | | |
| IV | DSE | Discipline Specific Elective II | Organic Chemistry of Natural Product | MCH2241 | 4 | 0 | 0 | 4 |
| | | | Photo-Inorganic Chemistry | MCH2242 | | | | |
| | | | Solid State: Theory & Applications | MCH2243 | | | | |
| | DSE | Discipline Specific Elective III | Polymer Chemistry | MCH2244 | 4 | 0 | 0 | 4 |
| | | | Chemistry of Nanomaterials and their Applications | MCH2245 | | | | |
| | OE | Open Elective I | Pharmaceuticals Chemistry | MCH2246 | 4 | 0 | 0 | 4 |
| | | | Environmental Chemistry | MCH2247 | | | | |
| | P | Project II | | MCH2248 | 0 | 0 | 16 | 8 |
| | Total Credits in Semester IV | | | | | | 20 | |
| Total Credits Over full Course | | | | | | 84 | | |

P: Project

A student at the end of the 2nd semester selects the faculty member as his/her MSc project/research guide. She/he will then work with the selected research guide for Project 1 and Project 2.

Project I: This is the first part of the project which is to be carried out in the university.

Project II: An intensive research work is to be carried out by the student under the guidance of an internal/external* research guide. At the end of the semester, a project report in the form of MSc dissertation has to be submitted in the Department of chemistry. The student also presents and defends his/her MSc dissertation to the committee constituted by the Head of the department. The committee will comprise of a research guide, two internal faculty members and Head.

*Internal research guide refers to faculty member of Department of chemistry, SRM University Sikkim. External research guide refers to faculty from other university.

Students pursuing project under external research guide may fulfil required credits (4th Semester) by taking online courses recognized by the university, for example SWAYAM, EDX etc.

List of Discipline Specific Electives and Open Elective courses

Discipline Specific Electives are offered to the students of chemistry. Students on their interest are free to take any electives from the list below.

Discipline Specific Elective

| Semester | Course Category | Course Name | Course Code | L | T | P | C |
|-----------------|------------------------|---|--------------------|----------|----------|----------|----------|
| III | DSE | Theoretical and Physical aspects of Organic Reactions | MCH2235 | 4 | 0 | 0 | 4 |
| | | Supramolecular chemistry and modern crystal engineering | MCH2236 | 4 | 0 | 0 | 4 |
| | | Computational Chemistry | MCH2237 | 4 | 0 | 0 | 4 |
| IV | DSE | Organic Chemistry of Natural Product | MCH2241 | 4 | 0 | 0 | 4 |
| | | Photo-Inorganic Chemistry | MCH2242 | 4 | 0 | 0 | 4 |
| | | Solid State: Theory & Applications | MCH2243 | 4 | 0 | 0 | 4 |
| IV | DSE | Polymer Chemistry | MCH2244 | 4 | 0 | 0 | 4 |
| | | Chemistry of Nanomaterials and their Applications | MCH2245 | 4 | 0 | 0 | 4 |

Open Elective (OE)

Open elective Courses offered by the Department of Chemistry is open to the students of all the department of the university. The courses are interdisciplinary in nature.

| Semester | Course Name | Course Code | L | T | P | C |
|-----------------|---------------------------|--------------------|----------|----------|----------|----------|
| IV | Pharmaceuticals Chemistry | MCH2246 | 4 | 0 | 0 | 4 |
| | Environmental Chemistry | MCH2247 | 4 | 0 | 0 | 4 |

List of proposed SWAYAM/EDX online courses

Students pursuing Project II (4th semester) under external faculty are requested to choose courses from the following approved list. Students have to fulfill **12 credits** in total. The details of the courses and the process of registration can be accessed by clicking <https://swayam.gov.in/>

| Semester | Course Name | Course Code | L | T | P | C |
|--------------------|---|-------------|---|---|---|---|
| Semester IV | A Study Guide in Organic Retrosynthetic: Problem Solving Approach | SWAYAM | - | - | - | 3 |
| | Essentials of Biomolecules : Nucleic Acids and Peptides | SWAYAM | - | - | - | 3 |
| | Advanced Transition Metal Organometallic Chemistry | SWAYAM | - | - | - | 3 |
| | Analytical Techniques | SWAYAM | - | - | - | 4 |
| | Approximate Methods in Quantum Chemistry | SWAYAM | - | - | - | 2 |

| Course Distribution | | | | | | |
|---------------------|--------------------|-------------------------------|----------------|-----------------------------|-----------|---------------|
| SEM | Core Courses (T+P) | Discipline Specific Electives | Open Electives | Ability Enhancement Courses | Project | Total Credits |
| I | 3(4)+3(2) | - | - | 1(2) | - | 20 |
| II | 4(4)+3(2) | - | - | - | - | 22 |
| III | 2(4)+2(3) + 1(2) | 4(1) | - | - | 2 | 22 |
| IV | - | 4(2) | 4(1) | - | 8 | 20 |
| Total | 56 | 12 | 4 | 2 | 10 | 84 |

Core: 66.67 %; DSE: 14.29 %; OE: 4.76 %; AEC: 2.38 %; Project: 11.90 %

SEMESTER I

| Course Category | Course Code | Course Name | L | T | P | C |
|--------------------------------------|--|--|---|---|---|---|
| CT | MCH2211 | Mechanistic Aspects of Organic Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome (CLO) | | | | | | |
| CLO1 | Illustrate organic reactions and their mechanisms. (B.L. - 2) | | | | | |
| CLO2 | Explain the reaction pathways of carbonyl compounds. (B.L. - 2) | | | | | |
| CLO3 | Apply the understanding of acid-base concepts in organic chemistry. (B.L. - 3) | | | | | |
| CLO4 | Distinguish the reactions as substitution and elimination. (B.L. - 4) | | | | | |
| CLO5 | Categorize reactions as addition and substitution reactions.(B.L. - 4) | | | | | |

Unit 1: Organic structures, reactions and conjugation

Structure of molecules – Introduction, atomic orbitals, Molecular orbitals, Bonding, Hybridization, Rotation and rigidity. (2 hours)

Organic reactions - Chemical reactions, Nucleophiles and electrophiles, Reaction mechanisms. (2 hours)

Nucleophilic addition to the carbonyl group - Molecular orbitals explanation about the reactivity of carbonyl group, Attack of cyanide on aldehydes and ketones, The angle of nucleophilic attack on aldehydes and ketones, Nucleophilic attack by ‘hydride’ on aldehydes and ketones. (2 hours)

Addition of organometallic reagents to aldehydes and ketones, Addition of water to aldehydes and ketones, Hemiacetals from reaction of alcohols with aldehydes and ketones, Ketones also form hemiacetals, Acid and base catalysis of hemiacetal and hydrate formation, Bisulfite addition compounds. (3 hours)

Delocalization and conjugation - The structure of ethene, Molecules with more than one C=C double bond, The conjugation of two π bonds, UV and visible spectra, The allyl system, Delocalization over three atoms is a common structural feature, Aromaticity. (3 hours)

Unit 2: Organometallic reagents, Nucleophilic substitution at the carbonyl group

Using organometallic reagents to make C–C bonds - Organometallic compounds, their synthesis, synthetic applications of organometallic compounds, Oxidation of alcohols. (3 hours)

Nucleophilic substitution at the carbonyl group - Nucleophilic addition to a carbonyl groups, Carboxylic acid derivatives, Tetrahedral intermediates, Carboxylic acid derivatives reactivity, Acid catalysts for carbonyl groups, Synthesis of acid derivatives, Ketones from esters. (5 hours)

Nucleophilic substitution at C=O with loss of carbonyl oxygen – Formation of hemiacetals and acetals from carbonyl compounds, Reaction of amines with carbonyl compounds, Imines: nitrogen analogues of carbonyl compounds. (4 hours)

Unit 3: pK_as, Equilibria, rates, mechanisms and Stereochemistry

Acidity, basicity, and pK_a - Organic compounds ions solubility in water, Acids, bases, and pK_a, Acidity, The definition of pK_a, constructing a pK_a scale. (1 hour)

Nitrogen compounds as acids and bases, Substituents affect the pK_a. (1 hour)

Carbon acids, pK_a in action—the development of the drug cimetidine, Lewis acids and bases. (2 hours)

Equilibria, rates, and mechanisms – Thermodynamics vs kinetics, Manipulation of equilibrium to favour the product of interest, Role of entropy in determining equilibrium constants, Variation of equilibrium constants with temperature. (2 hours)

Introducing kinetics: how to make reactions go faster and cleaner, Rate equations, Catalysis in carbonyl substitution reactions, Kinetic versus thermodynamic products. (2 hours)

Stereochemistry - Enantiomers, Diastereoisomers, Interconversion of Fischer and Sawhorse projection formula. (2 hours)

Chiral compounds with no stereogenic centres, Axes and centres of symmetry, Resolution. (2 hours)

Unit 4: Nucleophilic substitution, Conformational analysis, Elimination reactions

Nucleophilic substitution at saturated carbon - Mechanisms for nucleophilic substitution, Distinguishing S_N1 and S_N2 reaction mechanisms. (2 hours)

The leaving group in S_N1 and S_N2 reactions, The nucleophile in S_N1 reactions, The nucleophile in the S_N2 reaction, Comparison of Nucleophiles and leaving groups in S_N1 and S_N2 reaction. (2 hours)

Conformational analysis - Bond rotation and conformations, Conformation and configuration, Barriers to rotation. (2 hours)

Conformations of ethane, propane, butane; Ring strain, Cyclohexane, Substituted cyclohexanes. (2 hours)

Elimination reactions - Substitution and elimination, Elimination versus substitution, $E1$ and $E2$ mechanisms, Role of substrates and leaving group in $E1$ and $E2$ reaction. (2 hours)

Stereoselectivity in $E1$ reactions. Transition states in $E2$ eliminations, The regioselectivity of $E2$ eliminations, Anion-stabilizing groups allow another mechanism— $E1cB$. (2 hours)

Unit 5: Electrophilic addition, Substitution, Enols and enolates

Electrophilic addition to alkenes - Alkenes react with bromine, Oxidation of alkenes to form epoxides, Electrophilic addition to unsymmetrical alkenes and dienes, Regioselective opening of unsymmetrical bromonium ions. (2 hours)

Stereospecificity in electrophilic additions to alkenes, Dihydroxylation, Double bond cleavage: periodate cleavage and ozonolysis, Addition of water across a double bond. (2 hours)

Electrophilic aromatic substitution - Introduction: enols and phenols, Benzene and its reactions with electrophiles, Electrophilic substitution on phenols, anilines, Alkyl benzenes, halobenzenes, other monosubstituted phenyl derivatives, disubstituted phenyl derivatives, A closer look at Friedel–Crafts chemistry, Chemistry of the nitro group. (4 hours)

Formation and reactions of enols and enolates – Tautomerism, Evidence for the equilibration of carbonyl compounds with enols, Enolization catalysis by acids and bases, The enolate ion intermediate in the base-catalysed reaction, Types of enol and enolate, Stable enols, Consequences of enolization. (2 hours)

Reaction with enols or enolates as intermediates, Stable equivalents of enolate ions, Enol and enolate reactions at oxygen: preparation of enol ethers, Reactions of enol ethers. (2 hours)

Prescribed Books:

- (1) J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, 2nd edition, Oxford University Press, 2012.
- (2) D. Nasipuri, Stereochemistry of organic compounds principles and applications, New Age International Publishers, 2020.
- (3) John D. Hepworth, David R. Waring, Michael J. Waring, Aromatic Chemistry, Royal Society of Chemistry, 2002.
- (4) Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part A, Plenum Press, 2012.

Reference Books:

- (1) Ian Fleming, Molecular Orbitals and Organic Chemical Reactions, Student Edition, Wiley, 2009.
- (2) E. L. Eliel, S. H. Wilen, with a contribution by Lewis N. Mander, Stereochemistry of Organic Compounds, Wiley Student Edition, Reprint 2008.
- (3) W. J. Hehre, A. J. Shusterman, W. W. Huang, A Laboratory Book of Computational Organic Chemistry, Wavefunction Publications, 1998.
- (4) Michael B. Smith & J. March, Advanced organic chemistry, 6th Ed., John Wiley & Sons, Inc, NewYark, 2006.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|-----------------------------------|---|---|---|---|
| CT | MCH2212 | Principles of Inorganic Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Develop the knowledge of symmetry and point group in molecules and the role of symmetry in electronic spectroscopy. | | | | | |
| CLO2 | Capable to present the character table of simple molecules and their projection by SALC method. | | | | | |
| CLO3 | Gain the basic knowledge of magnetic properties of inorganic compounds and their explanations. | | | | | |
| CLO4 | Obtain the knowledge of application of magnetic properties of inorganic compounds. | | | | | |
| CLO5 | Acquire the knowledge of the preparation and structure of boron clusters and their applications. | | | | | |

Unit 1: Introduction to Symmetry and Group theory-I

Symmetry elements and operations, products of symmetry operations, equivalent symmetry elements. (2 hours)

The concept of groups; subgroups, classes and the related theorems; commutative (abelian) groups and cyclic groups and their examples. (1 hour)

Group multiplication tables and the rearrangement theory. (3 hours)

Identification of point groups, similarity transformation and the invariance of characters. (3 hours)

Matrix representation of symmetry operations. (2 hours)

Characters of symmetry operations in a representation. (3 hours)

The row/column orthogonality of characters, reducible and irreducible representations. (3 hours)

Unit 2: Symmetry and Group theory-II

Character tables (C_{2v} , C_{3v} , C_{4v} , D_4), (4 hours)

Representation for cyclic groups, wave functions as bases for Irreducible Representations, (3 hours)

The standard reduction formula; the direct product representation and its decomposition, (3 hours)

Identifying nonzero matrix elements, spectral transition probabilities, (2 hours)

Selection rules for IR and Raman transitions. (2 hours)

Projection operator (without derivation), use of the projection operator to form symmetry adapted linear combination (SALC) of simple system. (2 hours)

Unit 3: Magneto Chemistry I

Magnetic properties of substances, orbital and spin angular momentum of electrons, paramagnetic moment and magnetic susceptibility, zero-field splitting, spin-orbit coupling. (3 hours)

Paramagnetic and diamagnetic materials, ferromagnetism, ferrimagnetism, antiferromagnetism, magnetic permeability, magnetic susceptibility, magnetization, (2 hours)

Classical theory of diamagnetism and paramagnetism (Langevin's theory), (3 hours)

Determination of magnetic susceptibility by these methods: Gouy, Faraday and SQUID. (2 hours)

Unit 4: Magneto Chemistry II

Magnetic properties and temperature – The curie and Curie-Weiss law, derivation of Curie law. (2 hours)

Microstates, hole formalism, multiplet, multiplet width, Lande interval rule, magnetic moments for different multiplet widths, (2 hours)

Crystal field diagram, quenching of orbital contribution, high spin/low spin equilibrium (2 hours)

Mechanism like – direct interaction, superexchange interactions elucidation with poly nuclear metal complexes as well as oxide and halide salts of transition metals. (2 hours)

Unit 5: Clusters

Boron cluster classification, skeletal electron counting. Boron hydrides: boranes, structure, bonding (MO description of B_2H_6 and $B_2H_6^{2-}$) (4 hours)

Wade's rules, boron compounds of potential medicinal interest; boron neutron capture theory (BNCT). (2 hours)

Lipscomb's topology, "styx" system of numbering, nomenclature; carboranes, metalloboranes, metallocarboranes-synthesis and structure; (3 hours)

Prescribed Books:

- (1) Cotton, F.A., 1990 Chemical Applications of Group Theory Wiley Interscience, 3rd Ed, Wiley-Blackwell.
- (2) Magnetochemistry – Pierce W. Selwood, Swinburne Press, Australia, 2013. ISBN: 9781376175653, 9781376175653
- (3) Introduction to Magnetochemistry, Alan Earnshaw, Academic Press, New York, 2013.
- (4) Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 4th Edition, Pearson Publishers, 2006.

Reference Books:

- (1) Principles of Inorganic Chemistry, B. R. Puri, L. R. Sharma, K. C. Kalia, 33rd Edition, Vishal Publishing Co., India, 2020.
- (2) Concise Inorganic Chemistry, Lee, J. D., 5th Edition, Oxford University Press, 2008.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|-----------------------------|---|---|---|---|
| CT | MCH2213 | Thermodynamics and Kinetics | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | To develop the knowledge of laws of thermodynamics, its origin and implication in our daily life. | | | | | |
| CLO2 | To evaluate the thermodynamic parameters for micellization | | | | | |
| CLO3 | To develop the concept of irreversible thermodynamics for understanding Onsager's relation and electro-kinetic effect | | | | | |
| CLO4 | To acquire the fundamentals of statistical thermodynamics | | | | | |
| CLO5 | To develop and implement the theories of reaction kinetics for explaining different chemical reactions | | | | | |

Unit 1: Classical Thermodynamics and Phase equilibria

Review of laws of thermodynamics (1 hour)

Concept of Entropy, Clausius Inequality (1 hour),

Equations of states (1 hour),

Thermodynamic Maxwell relations (1 hour),

Free energy and Chemical potential (2 hours),

Partial molar quantities and their significances (2 hours),

Solution: Ideal and non-ideal, Raoult's law (1 hour),

Gibbs Phase rule (Derivation), Definition of Phase, component and Degree of freedom (2 hours),

Clausius-Clapeyron equation, Phase diagram of one, two (1 hour)

Three component systems (1 hour)

[13 Lectures]

Unit 2: Thermodynamics of Micelles

Surface active agents and their classification (2 hours)

Micellization, hydrophobic interaction (1 hour)

Critical micellar concentration (CMC), factors affecting CMC of surfactants (1 hour)

Counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models (2 hours)

Solubilisation, micro emulsions, and reverse micelles (1 hour).

[7 lectures]

Unit 3: Non Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states (1 hour),

Basic Postulates and Methodology (2 hours),

Onsager's Theory, Phenomenological Laws and Equations (2 hours),

Transformations of the generalized fluxes and forces (3 hours),

Microscopic Reversibility and Onsager's Reciprocal Relations (2 hours),

Entropy Production and entropy flow (2 hours),

Theorem of Minimum Entropy Production (2 hours),

Chemical Reactions, Coupled Reactions and Electro-kinetic Phenomena (3 hours).

[17 Lectures]

Unit 4: Statistical thermodynamics

Concept of distribution (1 hour),

Thermodynamic probability and most probable distribution (1 hour),

Ensemble averaging, postulates of ensemble averaging (1 hour),

Canonical, grand canonical and micro canonical ensembles (2 hours)

Corresponding distribution laws (using Lagrange's method of undermined multipliers) (2 hours)

Partition functions-translational, rotational vibrational and electronic partition functions (2 hours),

Calculation of thermodynamic properties (G, A) in terms of partition functions (2 hours).

Boltzmann Entropy (1 hour),

Heat capacity behaviour of solids – Einstein and Debye treatment (1 hour)

[13 Lectures]

Unit 5: Chemical Kinetics

Introduction to kinetics and concepts like order, Molecularity and integral equations (1),

Kinetic theory of collisions (1),

Rate theories based on thermodynamics and statistical mechanics-conventional transition state theory (2),

Thermodynamic formulation of conventional transition state theory - assumptions and limitations (1),

Microscopic reversibility (1),

Theories of unimolecular reactions- Lindemann theory, Lindemann-Hinshelwood mechanism, RRKM (2),

Composite reaction kinetics: Chain reactions (reaction between hydrogen (g) and Bromine (g)) and explosion reaction kinetics (H_2 and O_2) (2).

[10 Lectures]

Prescribed Books

- (1) P. W. Atkins, J de Paula, Physical Chemistry, 10th Ed, Oxford University Press, New Delhi (2018).
- (2) D. A. McQuarrie, J. D. Simon, Physical Chemistry: A Molecular Approach, 1st Edition: Viva Books ISBN: 8130919192 (1 January 2019).
- (3) Donald A. McQuarrie, Statistical Thermodynamics, University Science Books, U.S.; University Science Books; (2000)
- (4) Physical Chemistry, T. Engel and P. Reid, Pearson Education and Dorling Kindersley (India) (2006)
- (5) Kalidas and M.V.Sangaranarayan, Non-Equilibrium Thermodynamics, Principles and Applications, McMillanIndia Ltd., 2002
- (6) Sow Hsin Chen, Raj Rajagopalan, Micellar Solutions and Microemulsions: Structure, Dynamics, and Statistical Thermodynamics, Springer (2012)
- (7) I. Prigogine, Introduction to Thermodynamics of Irreversible Processes by, 3rd Ed. Interscience Publishers, 1967

Reference Books

- (1) Andrew Cooksy, Physical Chemistry: Thermodynamics, Statistical Mechanics, and Kinetics (2011) by 1st Edition
- (2) Thomas Engel and Philip Reid, Thermodynamics, Statistical Thermodynamics, & Kinetics: Pearson New International Edition 3rd Edition, (2012)
- (3) Hans-Jürgen Butt, Karlheinz Graf, Michael Kappl, Physics and Chemistry of Interfaces, Wiley 2003

- (4) R. Hasse, Thermodynamics of Irreversible Processes, Dover Publications Inc.; New edition (1 February 2000)

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|-------------------------|---|---|---|---|
| AEC | MCA2214 | Mathematics for Chemist | 2 | 0 | 0 | 2 |
| Course Learning Outcome | | | | | | |
| CLO1 | To Acquire the concepts on vectors, Matrices and Determinants | | | | | |
| CLO2 | To Implement differential calculus knowledge in evaluating derivatives of different functions | | | | | |
| CLO3 | To implement the knowledge of integral calculus in evaluating area of a given region | | | | | |
| CLO4 | To develop the understanding and solving different degree and order differential equations, Legendre transformation and power series | | | | | |
| CLO5 | To acquire the knowledge on Fourier series, transformations and probability | | | | | |

Unit I: Vectors, Matrices and Determinants

Matrix: addition and multiplication, inverse, Adjoint and transpose of matrices, special matrices (symmetric, skew symmetric, Hermitian, skew Hermitian, unit, diagonal, unitary etc.) and their properties, matrix equations: homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence, introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants, introduction to tensors.

[6 Lectures]

Unit II: Differential calculus

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials with their applications to thermodynamic properties.

[5 Lectures]

Unit III: Integral calculus

Basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations

[5 lectures]

Unit IV: Elementary differential equations

variables-separable and exact first-order differential equations, homogeneous, exact and linear equations, solutions of differential equations by the power series method, solutions of harmonic oscillator and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

[7 Lectures]

Unit V: Fourier series, Fourier Transforms and Probability

Fourier Series - Average Value of a Function - Fourier Coefficients – Fourier transformation, Dirichlet Conditions – Complex Form of Fourier Series - Other Intervals - Even and Odd Functions. Conditional probability, multiplication theorem on probability, independent events, total probability, Random variable and its probability distribution

[7 Lectures]

Prescribed Books

- (1) The chemistry Mathematics Book, E.Steiner, Oxford University Press (2008)

Reference Books

- (1) Basic Mathematics for Chemists, Tebbutt, Wiley (1994).
- (2) Mathematics for Chemists: Bhupendra Singh, Pragati Prakashan (2013).

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------------|--|------------------------------|---|---|---|---|
| CP | MCH2215 | Organic Qualitative Analysis | 0 | 0 | 4 | 2 |
| Course Learning Outcome (CLO) | | | | | | |
| CLO1 | To develop skills to separate binary mixtures of different classes of organic compounds and identify functional groups present in the individual components. | | | | | |
| CLO2 | To practice derivative preparation as a method to confirm presence of functional groups. | | | | | |
| CLO3 | To practice column chromatography for the separation of binary and ternary mixtures of organic compounds. | | | | | |
| CLO4 | To use Thin-Layer Chromatography for analysis of simple APIs available in market. | | | | | |
| CLO5 | Separate binary organic mixtures and identify functional groups in the components | | | | | |

(Mixture analysis & drug analysis)

1. Separation of mixtures containing TWO organic compounds and their characterisation by qualitative analysis.
2. TLC analysis of some patent medicines.

References

1. Elementary Practical Organic chemistry Part II, Qualitative Organic analysis by A.I. Vogel 2nd Ed, CBS publications, 1987.
2. Thin Layer chromatography - Laboratory Work book edited by Eigen Stahl, Springer International student edition, 1969.
3. Chromatography in Organic micro-analysis - A laboratory guide by Raphael Ikan, Academic press, 1982.
4. Quantitative analysis of Drugs in Pharmaceutical preparations by P.D. Sethi, 3rd Ed., CBS publishers, 1997.
5. Experimental Organic Chemistry by P.R. Singh, D.S. Gupta and K.S. Bajpai, Vols I & II, Tata Mc Graw Hill, 1980.

| Course category | Course Code | Course Name | L | T | P | C |
|-----------------|-------------|---|---|---|---|---|
| CP | MCH2216 | Estimation of metals present in alloy/mixture | 0 | 0 | 4 | 2 |

Separation and estimation of two metal ions from minerals, alloys or solutions.

1. Quantitative estimation of Zn(II) and Cu(II) in brass sample by volumetry and gravimetry 2B.
2. Quantitative estimation of iron in cast iron and steel.
3. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Mole-Ratio method.
4. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Slope-Ratio method.
5. Determination of composition of Fe(III)-sulfosalicylate complex in solution by Job's method of continuous variation.
6. Hydrothermal synthesis of metal-organic hybrid compounds and study on their physicochemical properties. Experiments will be set depending upon the availability of instruments and reagents.
7. Quantitative estimation of metal concentration at trace level by spectroscopic techniques (UV-Visible and atomic absorption spectroscopy).

Prescribed Books

- (1) Experimental Inorganic Chemistry - W. G. Palmer, 1954.
- (2) A text book of Quantitative Inorganic Analysis – A. I. Vogel, 1990.
- (3) Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall, 1970.

Reference Books

- (1) Handbook of Inorganic Synthesis: G. Brauer, 1965.
- (2) Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, University Science Books, 1999

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|--|---|---|---|---|
| CP | MCH2217 | Laboratory on Kinetics, polymer and phase equilibria | 0 | 0 | 4 | 2 |
| Course Learning Outcome | | | | | | |
| CLO1 | To implement the chemical kinetics theory in experiment. | | | | | |
| CLO2 | To determine Nernst Distribution law by determining the partition coefficient of iodine between water and carbon tetrachloride. | | | | | |
| CLO3 | To determine the CMC of surfactants through conductometer. | | | | | |
| CLO4 | To determining the molecular weight of a polymer | | | | | |
| CLO5 | To create the phase diagram of ternary system | | | | | |

List of Experiments

- (1) Determination of Partition coefficient of Iodine between water and Carbon tetrachloride
- (2) Phase diagram of ternary system ($H_2O/toluene/CH_3COOH$ or $H_2O/CH_3COCH_3/CHCl_3$)
- (3) Synthesis of silver nanoparticles by colloidal method and study of its optical properties
- (4) Determination of molecular weight of a polymer by viscometric method.
- (5) Determination of Critical Micelle Concentration (CMC) of a Surfactant by Conductometry
- (6) kinetics of the reaction between $K_2S_2O_8$ and KI , determine the rate constant and Order of the reaction, activation energy and study the influence of ionic strength on the rate constant
- (7) Study of kinetics of $KBrO_3 + KBr$ reaction - rate constant, activation energy and influence of ionic strength.
- (8) Determination of rates of hydrolysis of organic esters and verification of Hammett Equation.

Reference Books

1. C.D.Brennan and C.F.H.Tipper, A Laboratory Manual of Experiments in Physical Chemistry, McGraw-Hill, (2011).
2. F.Daniel & Others, Experimental Physical chemistry, Kogakasha CoLtd.,Tokyo (2001).

SEMESTER II

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|-----------------------------|---|---|---|---|
| CT | MCH2221 | Synthetic Organic Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Demonstrate chemo and regioselectivity in organic reactions using various protection-deprotection strategies. (B.L. 2) | | | | | |
| CLO2 | Extend the understanding of organic chemistry on heteroatom based organic molecules. (B.L. 2) | | | | | |
| CLO3 | Plans synthesis of natural products by retrosynthetic analyses. (B.L. 3) | | | | | |
| CLO4 | Examine the aromatic nature of heteroaromatic compounds. (B.L. 4) | | | | | |
| CLO5 | Examine the Stereoselective strategies available towards organic syntheses. (B.L. 4) | | | | | |

Unit 1: Conjugate addition and nucleophilic aromatic substitution, Chemoselectivity and protecting groups, Regioselectivity

Conjugate addition and nucleophilic aromatic substitution - Alkenes conjugated with carbonyl groups, Electrophilic nature of conjugated alkenes, Factors controlling conjugate addition, Extending the reaction to other electron deficient alkenes. (2 hours)

Conjugate substitution reactions, Nucleophilic epoxidation, Nucleophilic aromatic substitution, the addition–elimination mechanism. (1 hour)

The S_N1 mechanism for nucleophilic aromatic substitution: diazonium compounds. The benzyne mechanism. (1 hour)

Chemoselectivity and protecting groups – Selectivity, Reducing agents, Reduction of carbonyl groups, Hydrogen as a reducing agent: catalytic hydrogenation. (2 hours)

Removal of functional groups, dissolving metal reductions, Selectivity in oxidation reactions, competing reactivity. (1 hour)

A survey of protecting groups. (1 hour)

Regioselectivity - Regioselectivity in electrophilic aromatic substitution, Electrophilic attack on alkenes, Regioselectivity in radical reactions. (2 hours)

Nucleophilic attack on allylic compounds, Electrophilic attack on conjugated dienes, Conjugate addition, Regioselectivity applications. (2 hours)

Unit 2: Alkylation of enolates, Reactions of enolates with carbonyl compounds, Sulfur, silicon, and phosphorus in organic chemistry

Alkylation of enolates - Carbonyl groups show diverse reactivity, Some important considerations that affect all alkylations, Alkylations of nitriles and nitroalkanes, Choice of electrophile for alkylation, Lithium enolates of carbonyl compounds, Alkylations of lithium enolates. (3 hours)

Using specific enol equivalents to alkylate aldehydes and ketones, Alkylation of β -dicarbonyl compounds, Ketone alkylation regioselectivity, Enones-a solution to regioselectivity problems, Using Michael acceptors as electrophiles. (3 hours)

Reactions of enolates with carbonyl compounds: the aldol and Claisen reactions - The aldol reaction, Cross-condensations, Specific enol equivalents in control aldol reactions, Control aldol reactions of esters, aldehydes and ketones, Intramolecular aldol reactions. (3 hours)

Acylation at carbon, Cross ester condensations, Preparation of keto-esters by the Claisen reaction, Controlling acylation with specific enol equivalents, Intramolecular crossed Claisen ester condensations, Future of carbonyl chemistry. (3 hours)

Sulfur, silicon, and phosphorus in organic chemistry - Useful main group elements, Sulfur-stabilized anions, Sulfonium salts, Sulfonium ylids, Silicon and carbon compared, Allyl silanes as nucleophiles, The selective synthesis of alkenes, Dependence of properties of alkenes on their geometry, Exploiting cyclic compounds. (3 hours)

Equilibration of alkenes, Stereoselective addition to alkynes for formation of *E* and *Z* alkenes, Stereoselective elimination reactions, The Julia olefination, Stereospecific eliminations, Wittig reaction. (3 hours)

Unit 3: Retrosynthetic analysis

Creative chemistry, Retrosynthetic analysis: synthesis backwards, Synthons, Multiple step syntheses, Functional group interconversion, Two-group disconnections vs. one-group disconnections, C–C disconnections. (3 hours)

Donor and acceptor synthons, Two-group C–C disconnections, 1,5-Related functional groups, Natural reactivity and umpolung. (3 hours)

Unit 4: Heterocyclic compounds

Aromatic heterocycles 1: reactions - Pyridine an aromatic imine, Six-membered aromatic heterocycles with oxygen in the ring, Five-membered aromatic heterocycles and electrophilic substitution reactions on them, Furan and thiophene, More reactions of five-membered heterocycles, Five-membered rings with two or more nitrogen atoms, Benzo-fused heterocycles, Putting more nitrogen atoms in a six-membered ring, Fusing rings to pyridines: quinolines and isoquinolines, (6 hours)

Aromatic heterocycles 2: Synthesis, Disconnect the carbon–heteroatom bonds first, Pyrroles, thiophenes, and furans from 1,4-dicarbonyl compounds, The Hantzsch pyridine synthesis, Pyrazoles and pyridazines from hydrazine and dicarbonyl compounds, Pyrimidines from 1,3-dicarbonyl compounds and amidines, (3 hours)

Isoxazoles synthesis from hydroxylamine or by cycloaddition, Tetrazoles and triazoles synthesis by cycloadditions, The Fischer indole synthesis, Quinolines and isoquinolines, More heteroatoms in fused rings in synthesis. (3 hours)

Saturated heterocycles and stereoelectronics – Introduction, Reactions of saturated heterocycles, Conformation of saturated heterocycles, Making heterocycles: ring-closing reactions, Ring size and NMR, Geminal ($2J$) coupling, Diastereotopic groups. (6 hours)

Unit 5: Stereoselectivity

Stereoselectivity in cyclic molecules - Stereochemical control in six-membered rings, Reactions on small rings, Regiochemical control in cyclohexene epoxides, Stereoselectivity in bicyclic compounds, Fused bicyclic compounds, Spirocyclic compounds, Reactions with cyclic intermediates or cyclic transition states. (3 hours)

Diastereoselectivity – Prochirality, Diastereoselective additions to carbonyl groups, Stereoselective reactions of acyclic alkenes, Stereoselective Aldol reactions, Single enantiomers from diastereoselective reactions. (3 hours)

Prescribed Books

- (1) J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, Oxford University Press, Sec. Ed. 2012.
- (2) Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part A, Plenum Press, 2012.
- (3) J. March, Advanced organic chemistry, 6th Ed. Wiley - Interscience, 2006.
- (4) P.S. Kalsi, Organic reactions and mechanisms, 3rd Ed., New Age International Publishers 2010.

Reference Books

- (1) R.O.C. Norman, Principles of organic syntheses: 3rd Ed., Indian Reprint, Taylor and Francis Publishers, 2012.
- (2) Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part B, Plenum Press, 2012.
- (3) Michael B. Smith, Organic Synthesis, 4th Edition, Elsevier Publishers, 2016.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|-----------------------------|---|---|---|---|
| CT | MCH2222 | Applied Inorganic Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Explain the mechanism, kinetics and thermodynamics of reactions of coordination compounds. | | | | | |
| CLO2 | Develop the understanding of chemical bonding mostly based on Molecular Orbital Theory. | | | | | |
| CLO3 | Gain the knowledge of different types of organometallic catalysts, structures and their applications. | | | | | |
| CLO4 | Introduce the position of actinides and lanthanides in the periodic table, reasons for variable oxidation states, and various domestic, medical, industrial and military uses. | | | | | |
| CLO5 | Acquire the knowledge mechanism of different type of reactions. | | | | | |

Unit 1: Coordination Chemistry – I

Crystal field splitting diagrams in complexes of low symmetry; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions (4 hours)

Experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes, brief introduction to Angular Overlap Model. Electronic spectra of Transition Metal Complexes. (4 hours)

Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and Ni(II) complexes and calculation of ligand-field parameters (4 hours). Russell-Saunders coupling for d^n states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules. Spectral transition probability, vibronic coupling, non-centrosymmetric complexes, polarization of allowed transitions. (6 hours)

Unit 2: Coordination Chemistry – II

Co-ordination Chemistry-: Reactions, Kinetics and Mechanism, Substitution reactions in square planar complexes- rate law-trans effect mechanism (6 hours)

M –Ligand field effects and reaction rates- octahedral complexes mechanism- mechanism of redox reactions inner sphere and outer sphere complexes- electron transfer reactions- applications. (5 hours)

Unit 3: MOT and Inorganic Photochemistry

Molecular orbital treatment of co-ordination complexes. (3 hours)

Introduction to photochemical reactions, Laws of Photochemistry, Excited state metal complexes. (1 hours)

Jablonski Diagram. Relaxation processes of excited states- emission from excited states. Photo-substitution, photo-dissociation, photo-oxidation, photo-reduction and photo isomerism of complexes. (6 hours)

Unit 4: Bioinorganic Chemistry-I

Basic reactions in the biological system and the roles of metal ions. Role of alkali and alkaline earth metal ions in biology; Na^+ - K^+ -Pump, ionophores and crown ethers. Metal complexes in medicine- *cis*-platin, auranofin, Replication, Transcription & Translation of DNA. (4 hours)

Metal – nucleic acid Interactions-Metal ion interaction with Nucleosides & Nucleotides, Metal ion interaction with DNA, Metal ion interaction with RNA. (4 hours)

ATP-ADP Interconversion, Creatine- Phosphocreatine interconversion, phosphate transfer and its activation by metal ions. (4 hours)

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Unit 5: Bioinorganic Chemistry-II

Metallo Porphyrins- Dioxygen in Biological system- Reactions of molecular oxygen, Activation of Dioxygen Molecule in Transition Metal Dioxygen complexes. b) Oxygen carrying proteins- Hemoglobin & Myoglobin, Hemerythrin, Hemocyanin, cooperatively in haemoglobin, Bohr effect, Blood Substitute. (4 hours)

Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins. Model system- Synthetic oxygen carriers- Porphyrin Derivatives, Cobalt (II) Dioxygen complexes, Iridium (II) Dioxygen complexes (Vaska's complexes), Platinum group metal dioxygen complexes. (3 hours)

Redox enzymes- Molybdenum containing enzymes, Iron containing enzymes, Copper containing enzymes, Zinc containing enzymes Hydrolytic Enzyme-Carboxy peptidase, carbonic anhydrase Vitamins & co-enzymes. (3 hours)

Prescribed Books:

- (1) Huheey, J. 2006 Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York.
- (2) Lippard S.J & Berg J.M., Principles Of Bioinorganic Chemistry, panima publishing corporation, new delhi
- (3) Lee, J. D. 1999 Concise Inorganic Chemistry, Blackwell Science.
- (4) Shriver, D. F. and Atkins, P. W., 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
- (5) K.K Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2018, New Age International (P) Limited, Publishers.

Reference Books:

- (1) Principles of Inorganic Chemistry, 33rd Edition, B. R. Puri, L. R. Sharma, K. C. Kalia, Vishal Publishing Co., India.
- (2) Cotton, F.A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, New York.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|---|---|---|---|---|
| CT | MCH2223 | Principles, Theory and Applications of Spectroscopy | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Explain the theoretical principles of spectroscopy. (B.L. 2) | | | | | |
| CLO2 | Outline the theoretical aspects of Infrared and Microwave spectroscopy. (B.L. 2) | | | | | |
| CLO3 | Apply the principles of Raman spectroscopy, Electron Paramagnetic Resonance and Mossbauer spectroscopy. (B.L.3) | | | | | |
| CLO4 | Analyse and interpret the spectra given to determine the structure of organic molecules. (B.L.4) | | | | | |
| CLO5 | Infer the Circular Dichroism technique for Biology samples. (B.L.4) | | | | | |

Unit 1: Introduction to theoretical principles of Spectroscopy

A brief review of the selection rules for absorption of radiation by molecular vibrations, Intensity and line width of spectral line. Population of various states and intensity. Doppler broadening and life time broadening, factors affecting coupling, degeneracy. (4 hours)

Effect of co-ordination on spectra due to change in symmetry. (2 hours)

Basic outline of the instrumentation of microwave technique (2 hours)

Principles of Lasers. (2 hours)

Fermi's golden rule. (2 hours)

Unit 2: Theoretical aspects of Infrared and Microwave spectroscopy

Infrared spectroscopy - vibrations of polyatomic molecules- fundamental vibrations and their symmetry- overtone and combination frequencies- Fermi resonance. (2 hours)

The influence of rotation on the spectra of linear (polyatomic) molecules. (2 hours)

Effect of co-ordination on spectra due to change in symmetry. (2 hours)

Microwave spectroscopy – Rotation of molecules and rotational spectra - Diatomic molecules - the rigid rotor. (2 hours)

Intensity of spectral lines - effect of isotopic substitution. (1 hour)

Non-rigid rotator, spectrum of non-rigid rotator - poly atomic molecules - linear, symmetric top and asymmetric top molecules (only spectral features). (2 hours)

Basic outline of the instrumentation of microwave technique. (1 hour)

Unit 3: Principles of Raman spectroscopy, Electron Paramagnetic Resonance and Mossbauer spectroscopy

Raman Spectroscopy- Raman scattering - theory of Raman effect - pure rotational Raman spectra of linear, spherical, symmetric top and asymmetric top molecules. (2 hours)

Raman activity of vibrations - Structure determination CO_2 , N_2O , SO_2 , NO_3^- , ClO_3^- and ClF_3 using Raman spectroscopy. (2 hours)

Basic instrumentation. (3 hours)

Electron Paramagnetic resonance- Theory and applications to Nickel (II) & Copper (II) compounds, magnetic exchange process in di-nuclear complexes. (3 hours)

Mossbauer spectroscopy- Origin and interpretation of Mossbauer Effect- Mossbauer chemical shift. Application of Mossbauer spectroscopy to Fe and Sn systems. (2 hours)

Unit 4: Application of U.V., N.M.R. and Mass Spectroscopy in organic chemistry

Use of shift reagents – in U.V. spectral analysis, with examples chosen from chemistry of naturally occurring flavonoids- where such methods have been particularly successful. (2 hours)

I.R. spectra with regards to study of hydrogen bonding and resonance effects in organic compounds. (1 hour)

Advanced aspects of NMR: Use of paramagnetic shift reagents. (1 hour)

NOE effect, FT NMR its advantage. (1 hour)

Double resonance, with particular reference to spin - spin decouplings, solvent effects in PMR spectra. (2 hours)

^{13}C NMR – Introduction and theory. (1 hour)

Two dimensional NMR spectroscopy:

Introduction - Theory and applications of DEPT spectra and Homo COSY. (1 hour)

Applications of Hetero COSY- HMQC and HSQC. (1 hour)

Incredible natural abundance double quantum transfer experiment (2-D INADEQUATE) - Problem solving. (1 hour)

Applications of NMR Spectroscopy- in inorganic chemistry with special reference to ^{31}P , ^{19}F , ^{11}B nuclei and NQR spectroscopy. (2 hours)

Mass spectrometry- High resolution mass spectral fragmentation mechanism, soft ionization techniques. (1 hour)

Applications. (1 hour)

Combined problem solving- extensive analysis of problems based on integrated spectral data with examples chosen from natural products. (3 hours)

Unit 5: Circular Dichroism technique for Biology samples

CD of proteins, peptide conformations, DNA-protein and protein- protein interactions. (2 hours)

Basic outline of the instrumentation of microwave technique. (2 hours)

Basic instrumentation. (1 hour)

Basic outline of the instrumentation of microwave technique. (1 hour)

Prescribed Books:

- (1) Pavia, Lampman and Kriz, Introduction to Spectroscopy, A Guide to students of Organic Chemistry, 5th Ed, 2014.
- (2) C.N. Banwell, Fundamentals of Molecular Spectroscopy, 3rd Ed., T.M.H. Publishing Co 2017.
- (3) Silverstein, Bassler and Morrill, Spectrometric identification of Organic Compounds, 6th Ed., Wiley, 2013.

Reference Books:

- (1) Horst Friebolin, Basic One and Two-Dimensional NMR Spectroscopy, 5th Ed. Wiley-VCH, 2011.
- (2) Kensl E. Van Holde, W. Curtis Johnson, P. Shing Ho, Principles of Physical Biochemistry, 2nd Ed., Pearson Prentice Hall, 2005.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|---|---|---|---|---|
| CT | MCH2224 | Quantum Chemistry and Solid state Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | To develop the mathematical foundation for solving Quantum model systems | | | | | |
| CLO2 | To implement variational principles and perturbation theory in understanding stark effect, light matter interaction and anharmonic oscillator problems | | | | | |
| CLO3 | To analyze MO theory on the basis of Quantum mechanics | | | | | |
| CLO4 | To understand the quantum chemistry of many electron system | | | | | |
| CLO5 | To implement XRD pattern of the solids in understanding their crystal structures | | | | | |

Unit 1: Foundation of Quantum mechanics and model systems

Historical development (1 hour),

Operator algebra (1 hour),

Postulates of Quantum mechanics,

Born interpretation of a wave function (1 hour),

Schrödinger equation, Stationary states (1 hour)

Model systems:

- (a) Free-particle and particle in 1D, 2D and 3D box (1 hour),
- (b) Harmonic oscillator problem, Ladder operators, Power Series method, Hermite polynomial (2 hours)
- (c) Rigid rotator problem, Angular momentum operators (2 hours)
- (d) Hydrogen atom problem: Quantum numbers, Orbitals and energy (3 hours)

Concept of Quantum tunnelling with example (1 hour)

[13 Lectures]

Unit 2: Approximate method in Quantum chemistry

The variation method – Eckart's theorem (1 hour),

Examples of variational calculation, Linear Variation method (2 hours),

The perturbation theory – Time dependent and time independent, degenerate and non-degenerate (4 hours)

Example problem (stark effect, perturbed particle in a box, anharmonic oscillator) (5 hours)

[12 lectures]

Unit 3: Quantum mechanical treatment of diatomic molecules

The Born–Oppenheimer Approximation (1 hour),

Nuclear Motion in Diatomic Molecules, Atomic Units, Hydrogen Molecule Ion (2 hours),

Approximate Treatments of the H_2^+ Ground Electronic State (2 hours),

Molecular Orbitals for H_2^+ Excited States (1 hour),

MO Configurations of Homonuclear-Diatomic Molecules, Electronic Terms of Diatomic Molecules (2 hours),

The Hydrogen Molecule, The Valence-Bond Treatment of H_2 (1 hour),

Comparison of the MO and VB Theories, MO and VB Wave Functions for Homo-nuclear Diatomic Molecules, Excited States of H_2 (3 hours)

[12 Lectures]

Unit 4: Electron spin and Quantum mechanical treatment of many electron atoms

Electron spin, Stern-Gerlach experiment (1 hour),

Pauli's Antisymmetry principle, Slater determinant for many electrons systems (1 hour),

Fermions and Bosons (1 hour),

Pure spin states and energy expectation value of pure spin state (2 hours), Orbitals in many electron atoms: Hartree-Fock Theory, Total energy and Koopmans's theorem (2 hours);

Matrix formulation of Hartree-Fock, Roothaan (1 hour);

Ground state electronic configuration of elements, Spectroscopic term symbols (2 hours):

Vector model of an atom; LS, JJ coupling, electronic spectrum of many electron atoms, Zeeman Effect in many electron atoms (3 hours)

[13 Lectures]

Unit 5: Solid State chemistry

Crystal structure, Lattice planes, Miller indices, Reciprocal lattice, Brillouin Zones, Crystal system (3 hours),

Symmetry elements, Point groups and Space group (introductory) (2 hours),

X-ray direction, Bragg's law, X-ray diffraction, indexing of peaks (3 hours),

Important Crystal structure type: Rock Salt, Zinc blende, Diamond, Wurtzite, Perovskite (2 hours)

[10 Lectures]

Prescribed Books

- (1) David J. Griffiths, Introduction to Quantum Mechanics, Cambridge India (2016)
- (2) Ira N Levine, Quantum Chemistry, Pearson 7th Edition (2016)
- (3) Donald A McQuarrie, Quantum Chemistry, University Science Books, U.S (2007)
- (4) AB Sannigrahi, Quantum Chemistry, First edition, Arunabha Sen Books & allied (P) Ltd (2007).

Reference Books

- (1) A. K. Chandra, Introductory Quantum Chemistry 4th Edition (2017)
- (2) A Szabo and Neil S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory Dover (2001)

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|---|---|---|---|---|
| CP | MCH2225 | Organic Synthesis (multistep) and Spectral Analysis | 0 | 0 | 4 | 2 |
| Course Learning Outcome | | | | | | |
| CLO1 | To give hands-on experience in carrying out various types of organic reactions including addition, elimination, condensation and functional group protection reactions. | | | | | |
| CLO2 | Gain the skills and expertise to design and carry out organic reactions performed during the course and use it in multi-step organic synthesis. | | | | | |

Design and synthesis of organic compounds possessing novel features.

Experiments involving - enamine reactions, Robinson annelation, Wittig reaction and protection - deprotection sequence (use of cyclic acetals in the protection of carbonyl - use of ester in the protection of alcohols or phenols etc.,)

Preparative organic photochemistry - preparation of phenanthrene - 9-carboxylic acid and benzpinacol.

Use of polymer supported organic synthesis (Silica supported reagents, alumina supported reagents etc.)

Zeisel's estimation, Zeriwittinoff's estimation

References:

- (1) Experimental technique in Organic Chemistry by D.J Pasto, C.R.Johnson and M.J.Miller, Prentice Hall, 1992.
- (2) Experimental Organic Chemistry: Principles and Practice by L. M. Harwood and C.J. Moody, Blackwell Scientific Publications, 1989
- (3) Reactions and Syntheses by L.F. Tietze and Th. Eicher, University Science Books, California, 1989.
- (4) Vogel's Textbook of Practical Organic Chemistry revised by B. S. Furniss et al., 5th Ed., ELBS, 1989.

| Course category | Course Code | Course Name | L | T | P | C |
|-----------------|-------------|---|---|---|---|---|
| CP | MCH2226 | Synthesis and Characterization of inorganic compounds | 0 | 0 | 4 | 2 |

Synthesis and Characterization of inorganic compounds (Any Five)

1. Reinkey's salt
2. Tris(2,2'-bipyridine)ruthenium (II) perchlorate
3. $[\text{Cu}(\text{NH}_3)_4(\text{SO}_4)(\text{H}_2\text{O})]$
4. $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$
5. $[\text{Ni}(\text{en})_2]\text{Cl}_2$
6. $\text{K}_3[\text{Fe}(\text{ox})_3]$
7. Tris (acetylacetonato) iron (III)
8. $[\text{Cu}(\text{NH}_3)_4(\text{SO}_4)(\text{H}_2\text{O})]$
9. Crome alum $[\text{K}_2\text{SO}_4, \text{Cr}_2(\text{SO}_4)_3, 24\text{H}_2\text{O}]$
10. Porphyrin Metal Complexes
11. Pthalocyanin Metal complexes

Prescribed Books

- (1) Experimental Inorganic Chemistry - W. G. Palmer, 1970.
- (2) A text book of Quantitative Inorganic Analysis – A. I. Vogel, 1990.
- (3) Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall, 1970.

Reference Book

- (1) Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, University Science Books, 1999.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------------|---|---|---|---|---|---|
| CP | MCH2227 | Laboratory on electrochemistry and spectroscopy | 0 | 0 | 4 | 2 |
| Course Learning Outcome (CLO) | | | | | | |
| CLO1 | To design experiments with better sample preparation for accurate analysis | | | | | |
| CLO2 | To handle sophisticated equipment for different chemical analysis. | | | | | |
| CLO3 | understand the principles behind the physical chemistry experiments perform and be in a position to explain them | | | | | |
| CLO4 | measure various kinetic parameters in different chemical systems and solve problems based on rate/rate constants for different types of reactions | | | | | |

List of Experiments

1. Manganese determination by titrating with permanganate in neutral pyrophosphate Solution.
2. Estimate concentration of H_2SO_4 , CH_3COOH and CuSO_4 by conductometric titration with NaOH .
3. Titration of pure solutions of KI , KCl and KBr and their mixtures against AgNO_3 .
4. Fluorescence quenching experiment: Determination of rate constant for fluorescence quenching of Alq_3 (or any other fluorophore) by acrylamide, urea, Br^- and I^-
5. Thermodynamics experiment: Determination of enthalpy and entropy of excimer formation (e.g. pyrene or some other appropriate fluorophore)
6. Kinetic salt effect: To study the kinetics of reduction of Maxilon Blue-SG by sulfide Ion
7. Nanoparticle growth kinetics: Study of nanoparticle growth kinetics in zinc oxide using UV-Visible spectroscopy
8. Activation energy determination: Study of the kinetics of ethylacetate hydrolysis by NaOH using conductance measurements and determination of the energy of activation of the

reaction

9. Enzyme kinetics: Study of enzyme kinetics: hydrolysis of esters by α -chymotrypsin and the Michaelis-Menten equation

Reference Books:

- (1) Donald T. Sawyer, William R. Heineman & Jalice M. Beebe, Chemistry experiments for Instrumental Methods, John Wiley & Sons, 1984.
- (2) Vogel's Textbook of Quantitative Chemical Analysis (revised copy) 5th Ed., ELBS, 1994.
- (3) G. Peter Matthews, Experimental Physical Chemistry, Clarendon Press, 1985.
- Neidig and Strattom,
- (4) Modern Experiments for Introductory Chemistry, 2nd Ed., Reprinted from Journal of Chemical Education, 1989.
- (5) G. Peter Matthews, Experimental Physical Chemistry, Clarendon Press, 1987.
- (6) A. M. Halpern, Experimental Physical Chemistry, 3rd Ed., W. H. Freeman, 2006

SEMESTER III

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|-----------------------------------|---|---|---|---|
| CT | MCH2231 | Implications of Organic Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Outline various aspects of Photochemistry and Pericyclic reactions. (B.L. 2) | | | | | |
| CLO2 | Explain Participation, Rearrangement, Fragmentation, Radical reactions. (B.L. 2) | | | | | |
| CLO3 | Apply the concepts of reaction intermediates in the chemistry of carbenes, nitrenes and Determining reaction mechanisms. (B.L. 3) | | | | | |
| CLO4 | Discover the newer dimension of organic chemistry, <i>i.e.</i> Organometallics and asymmetric synthesis. (B.L. 4) | | | | | |
| CLO5 | Extrapolate the organic chemistry in the biological systems and frontier areas. (B.L. 4) | | | | | |

Unit 1: Photochemistry and Pericyclic reactions

Organic Photochemistry: Alkenes, isomerization, cycloaddition, di- Π methane reaction, ring closure - carbonyl compounds, Norrish type I & II reactions, Paterno-Buchi reaction - aromatic photochemistry, isomerizations, photoaddition, cycloadditions to the aromatic ring - singlet oxygen oxidations. (2 hours)

Pericyclic reactions: cycloadditions- General description of the Diels–Alder reaction, The frontier orbital description of cycloadditions, Regioselectivity in Diels–Alder reactions, The Woodward–Hoffmann description of the Diels–Alder reaction, Trapping reactive intermediates by cycloadditions, Other thermal cycloadditions. (3 hours)

Photochemical [2 + 2] cycloadditions, Thermal [2 + 2] cycloadditions Making five-membered rings: 1,3-dipolar cycloadditions, Two very important synthetic reactions: cycloaddition of alkenes with osmium tetroxide and with ozone. (2 hours)

sigmatropic and electrocyclic reactions - Sigmatropic rearrangements, Orbital descriptions of [3,3]-sigmatropic rearrangements, the direction of [3,3]-sigmatropic rearrangements, [2,3]-Sigmatropic rearrangements, [1,5]-Sigmatropic hydrogen shifts. (3 hours)

Electrocyclic reactions. (2 hours)

Unit 2: Participation, Rearrangement, Fragmentation, Radical reactions

Participation - Neighbouring groups participation in acceleration of substitution reactions, Rearrangements due to neighbouring group participation (2 hours)

Rearrangement - Carbocations rearrangement, The pinacol rearrangement, The dienone-phenol rearrangement, The benzilic acid rearrangement, The Favorskii rearrangement, Migration to oxygen: the Baeyer–Villiger reaction, The Beckmann rearrangement (2 hours)

Fragmentation - Polarization of C–C bonds in fragmentation, Control in fragmentations by stereochemistry, Ring expansion by fragmentation, Controlling double bonds using fragmentation, The synthesis of Nootkatone: fragmentation showcase (2 hours)

Radical reactions – Radicals formation and stability, Radicals structure analysis, Radical–radical reactions, Radical chain reactions. (2 hours)

Chlorination of alkanes, Allylic bromination, Reversing the selectivity: radical substitution of Br by H, Carbon–carbon bond formation with radicals, The reactivity pattern of radicals. (2 hours)

Alkyl radicals from boranes and oxygen 998 Intramolecular radical reactions are more efficient than intermolecular ones. (2 hours)

Unit 3: Synthesis and reactions of carbenes, nitrenes and Determining reaction mechanisms

Synthesis and reactions of carbenes – Synthetic utility of Diazomethane, Photolysis of diazomethane to carbene, evidences of carbenes. (2 hours)

Carbenes synthesis, Classification of Carbenes, Mechanism of carbenes reactions - Carbenes reactions with alkenes, Insertion into C–H bonds, Rearrangement reactions. (2 hours)

Nitrenes - nitrogen analogues of carbenes, Alkene metathesis. (2 hours)

Determining reaction mechanisms - Determining reaction mechanisms: the Cannizzaro reaction, Product analysis, Systematic structural variation. (2 hours)

The Hammett relationship, Other kinetic evidence for reaction mechanisms, Acid and base catalysis. (2 hours)

The detection of intermediates, Stereochemistry and mechanism. (2 hours)

Unit 4: Organometallic chemistry and Asymmetric synthesis

Organometallic chemistry - Transition metals in organic reactions, The 18 electron rule, Bonding and reactions in transition metal complexes. (2 hours)

Palladium metal in homogeneous catalysis, The Heck reaction, Cross-coupling of organometallics and halides, Activation of allylic electrophiles by palladium (0), Palladium-catalysed amination of aromatic rings. (2 hours)

Alkenes coordinated to palladium(II) are attacked by nucleophiles, Palladium catalysis in the total synthesis of a natural alkaloid, An overview of some other transition metals. (2 hours)

Asymmetric synthesis - The chiral pool: Nature's chiral centres. (2 hours)

Resolution to separate enantiomers, Chiral auxiliaries, Chiral reagents (2 hours)

Asymmetric catalysis, Asymmetric formation of carbon-carbon bonds, Asymmetric aldol reactions, Enzymes as catalysts, factors responsible for enzyme efficiency (Bruice's proximity effect, Koshland's Orbital steering, Multifunctional catalysis). (2 hours)

Unit 5: Organic chemistry of life and Organic chemistry today

Organic chemistry of life - Primary metabolism, Nucleic acids as genetic information carrier. (2 hours)

Proteins structure, Sugars—biological importance, Lipids, Mechanisms in biological chemistry. (2 hours)

Natural products, Fatty acids and other polyketides from acetyl CoA, Terpenes - volatile constituents of plants. (2 hours)

Organic chemistry today - Science advances through interaction between disciplines. (2 hours)

Chemistry vs viruses. (2 hours)

The future of organic chemistry. (2 hours)

Prescribed Books:

- (1) J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, Oxford University Press, Sec. Ed. 2012.
- (2) Nicholas J. Turro, V. Ramamurthy, Juan Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Book Publishers, 2010.
- (3) Ian Fleming, Molecular Orbitals and Organic Chemical Reactions, Student Edition, Wiley, 2009.
- (4) Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part A, Plenum Press, 2012.

Reference Books:

- (1) Carey and Sundberg, Advanced organic chemistry, 5th. Ed., Part B, Plenum Press, 2012.
- (2) Raymond. K. Mackie, David M. Smith, R. Alan Aitken, Guidebook to Organic Synthesis, Prentice Hall Publishers, 3rd edition, 1999.
- (3) W. Carruthers, Iain Coldham, Modern Methods of Organic Synthesis South Asia Edition, Cambridge University Press, 2015.
- (4) Sunil Kumar, Vinod Kumar, S. P. Singh, Pericyclic Reactions: A Mechanistic and Problem Solving Approach, 1st Edition, Elsevier Publishers, 2015

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|---|---|---|---|---|
| CT | MCH2232 | Chemistry of <i>d</i> and <i>f</i> block elements | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Provide a thorough understanding of the relationship between the structures, chemical bonds and chemical properties in organometallic chemistry. | | | | | |
| CLO2 | Gain the knowledge of different types of organometallic catalysts, structures and their applications. | | | | | |
| CLO3 | Acquire the knowledge mechanism of different type of reactions. | | | | | |
| CLO4 | Acquire the fundamental knowledge of different types of nuclear reaction mechanism. | | | | | |
| CLO5 | Introduce the position of actinides and lanthanides in the periodic table, reasons for variable oxidation states, and various domestic, medical, industrial and military uses. | | | | | |

Unit 1: Organometallic Chemistry –I

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, (3 hours)

Ligands in organometallic chemistry; Synthesis, bonding and reactivity of Metal-alkyl, -alkene, -alkyne, -allyl, -carbene, -carbyne and -carbide complexes, (4 hours)

Agostic interaction, Stereochemical non-rigidity and fluxional behavior of organometallic compounds with typical examples. (3 hours)

Unit 2: Organometallic Chemistry –II

Chemistry of transition metal complexes with cyclic polyenes: 3-6 membered ring systems. Sandwich and non Sandwich complexes. (2 hours)

Organometallic chemistry of heterocyclic ligands (N, B, O). (2 hours)

Multidecker Sandwich complexes. Bioorganometallic chemistry, organometallic polymers, Main group organometallic chemistry. (2 hours)

Terminology in catalysis: TO, TON, TOF. Unique reactions in organometallic chemistry and catalysis: Coordinative unsaturation, Substitution, Oxidative addition, Insertion (migration), Isomerization, Reductive elimination; (2 hours) Catalytic converters; Alkene hydrogenation, Water gas shift reaction, Fischer Tropsch process. Hydroformylation (Oxo process), (2 hours) Carbonylation of olefins, Monsanto's acetic acid synthesis, Wacker oxidation (Pd-catalyzed), Polymerization of olefins, Ziegler-Natta catalyst. (4 hours)

Unit 3: Inorganic Reaction Mechanism

Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, different types of mechanisms (D, A, I_a and I_d). (2 hours)

Techniques for experimental measurements of reaction rates, techniques for fast reaction (2 hours)

Substitution reactions: Application of CFT, mechanism of ligand substitution in octahedral complexes, mechanism of isomerization and racemization, substitution reactions in square planar complexes. Cis- and trans- effects. (2 hours)

Mechanism of redox reactions with reference to metal complexes. (2 hours)

Electron transfer reactions – outer sphere and inner sphere, induced electron transfer reactions, two electron transfer reactions, non-complementary reactions, (2 hours)

Electroprotic reactions, Twist mechanism of racemization, inversion of configuration and associated process. (2 hours)

Unit 4: Nuclear Chemistry

Nuclear models-nuclear forces, liquid drop model, Fermi gas model, Magic numbers. (4 hours)

Nuclear spin and nuclear isomerism. (2 hours)

Nuclear reactions-energetics, mechanism and models, nuclear fission and nuclear fusion. (2 hours)

Nuclear reactors and particle accelerators. (2 hours)

Interaction of radiation with matter. (2 hours)

Unit 5: Lanthanides and Actinides

Lanthanides. Actinides and Super heavy elements. (1 hour)

Electronic structure, differences between $4f$ and $5f$ orbitals. (2 hours)

Stable oxidation states. Lanthanide and Actinide contraction, separation and isolation. (1 hour)

Absorption spectra and magnetic properties. (2 hours)

Comparative chemistry of d and f block elements, Comparative chemistry of Lanthanides and Actinides. (2 hours)

Aqueous chemistry, coordination chemistry. (2 hours)

Organometallic compounds lanthanides, trans actinide elements, (2 hours)

Periodicity of trans Lawrencium elements, super actinides. (2 hours)

Prescribed Books:

(1) Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, 6th Edition, John Wiley & Sons, New York, 2017.

(2) Concise Inorganic Chemistry, J. D. Lee, 5th Edition, Wiley India Pvt. Ltd, 2014.

(3) Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 4th Edition, Pearson Publishers, 2006.

(4) Basic Organometallic Chemistry, Anil Elias, B. D. Gupta, Universities Press, 2nd Edition, 2013.

(5) Nuclear and Radiochemistry: Fundamentals and Applications, Jens-Volker Kratz, 4th Edition, John Wiley & Sons, New York, 2022.

(6) Nuclear and Radiochemistry, Jozsef Konya, Noemi Nagy, 2nd Edition, Elsevier, 2018.

Reference Books:

(1) Principles of Inorganic Chemistry, B. R. Puri, L. R. Sharma, K. C. Kalia, 33rd Edition, Vishal Publishing Co., India, 2020.

(2) Radiochemistry and Nuclear Chemistry, Gregory Choppin, Jan-Olov Liljenzin, Jan Rydberg, Elsevier Science & Technology, 3rd Edition, 2001.

(3) Lanthanide and Actinide Chemistry, Simon Cotton, Wiley, 1st edition, 2006.

| Course category | Course Code | Course Name | L | T | P | C |
|-----------------|--|---|---|---|---|---|
| CT | MCH2233 | Fundamentals and applications of Electrochemistry | 3 | 0 | 0 | 3 |
| CLO1 | To explain the unique perspectives that statistical treatment of data brings to the study of chemistry (B.L. 2) | | | | | |
| CLO2 | To understand chromatographic separations and solvent extractions (B.L. 2) | | | | | |
| CLO3 | To study various advanced separation techniques crucial for both qualitative and quantitative analysis of samples (B.L. 3) | | | | | |
| CLO4 | To extend existing electro-analytical methods to new types of samples, and to learn about their applications in the areas of photoelectron chemistry. (B.L. 4) | | | | | |
| CLO5 | To study the instrument layout and understand the working of various components of instruments (B.L. 4) | | | | | |

Unit 1: Basic electrochemistry

Arrhenius theory of electrolytic dissociation (2 hours),

Molar conductivity at infinite dilution (2 hours),

Kohlrausch law of independent migration of ions (2 hours),

Debye-Hückel-Onsager equation derivation (3 hours),

rules of oxidation/reduction of ions based on half-cell potentials (2 hours),

Chemical cells, reversible and irreversible cells with examples (1 hour),

Electromotive force of a cell and its measurement (2 hours),

Nernst equation (3 hours);

Standard electrode (reduction) potential and its application to different kinds of half-cells (2 hours), pH values (1 hour), using hydrogen, Quinone-hydroquinone, glass electrodes (1 hour).

Unit 2: Ionics

Electrochemistry of solution (1 hour),

Debye-Huckel theory with derivation (3 hours),

Electrolytic conductivity and its types (1 hour),

Debye- Huckel – Onsagar treatment and its extension with derivation (1 hour)

Unit 3: Electrodictics

The concept of over potential, type of over-potentials: Origin and Minimization; exchange current density (1 hour),

Electrochemical reaction under charge transfer control, basic electrodictic equation (2 hours), Butler-Volmer equation- Derivation (2 hours),

The current potential Laws at other types of charges interfaces (1 hour),

Electrode reaction and chemical reaction- multistep reactions, transient behaviour of interfaces (1 hour),

Determining the step wise mechanism of an electrodictic reaction, current potential laws for electrochemical systems (1 hour)

Unit 4: General applications of electrochemistry

Electrodictic reaction of special interest- electrocatalysis- influence of various parameters (1 hour),

Photo electrochemistry: Introduction to Band bending at the semiconductor/solution interface- photoexcitation of electron by absorption of light-surface effects in photo- electrochemistry (2 hours),

Application of Butler-Volmer equation in corrosion, Tafel Equations (2 hours),

determination of kinetic parameters (1 hours)

Unit 5: Application in Electrochemical energy and sensing

Electrochemistry energy conversion- electricity storage, batteries, supercapacitors, fuel cells, Enzymes as electrode, Electrochemical sensors- electrochemical biosensors (1 hour),

gas sensors- solid state devices and sensor arrays (1 hour).

Electrochemical Impedance spectroscopy (1 hour),

complex variables, development of kinetic models, modeling with equivalent circuit analogues (1 hour).

Prescribed books:

- (1) Peter Atkins, Julio de Paula, James Keeler, Physical Chemistry 11th Edition, Oxford University Press, Oxford, 2018.
- (2) Allen J Bard, Larry R Faulkner, Henry S. White, Electrochemical Methods – Fundamentals and Applications, John Wiley & Sons, Limited, 2020.

Reference books:

- (1) Normand M. Laurendeau, Statistical Thermodynamics: Fundamental and Applications, Cambridge University Press, Cambridge, 2005.
- (2) Biman Bagchi, Statistical mechanics for chemists and materials science, CRC Press, Taylor and Francis Group 2019.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|----------------------|---|---|---|---|
| CT | MCH2234 | Analytical Chemistry | 3 | 0 | 0 | 3 |
| Course Learning Outcome | | | | | | |
| CLO1 | To explain the unique perspectives that statistical treatment of data brings to the study of chemistry (B.L. 2) | | | | | |
| CLO2 | To understand chromatographic separations and solvent extractions (B.L. 2) | | | | | |
| CLO3 | To study various advanced separation techniques crucial for both qualitative and quantitative analysis of samples (B.L. 3) | | | | | |
| CLO4 | To extend existing electroanalytical methods to new types of samples, and to learn about their applications in the areas of photoelectron chemistry. (B.L. 4) | | | | | |
| CLO5 | To study the instrument layout and understand the working of various components of instruments (B.L. 4) | | | | | |

Unit 1. Evaluation of Analytical Data

The uses of Statistics – the standard deviation of computed results (1 hour)

Method of least squares (1 hour),

Methods for reporting analytical data (1 hour),

Confidence intervals, Introduction to Error Analysis, Instruments Architecture and methods of detection (2 hours).

Unit 2. Separation Techniques

Super critical fluid chromatography- Principle and instrumentation-Applications of SCF (2 hours),

Super critical extraction chromatography: Principles, advantages and applications (2 hours),

Capillary electrophoresis - Capillary electro-chromatography (2 hours),

Solvent extraction - Multiple batch extraction, Counter-current distribution (2 hours),

Solid phase extraction - flow injection analysis - reverse osmosis, electro-dialysis, Affinity chromatography (2 hours),

Ultra-High-Performance Liquid Chromatography (UHPLC), Pyrolysis gas chromatography; Fast Protein Liquid Chromatography (2 hours)

Unit 3. Electroanalytical Methods

Different types of electrodes, mercury electrode, solid electrodes, chemically modified electrodes and microelectrodes (3 hours),

Voltammetry - pulse voltammetry (normal, differential, square wave, stair case voltammetry), AC voltammetry (3 hours),

chronoamperometry-bi-amperometry, Cyclic Voltammetry (2 hours),

Stripping Methods (anodic, cathodic, and adsorptive) and applications. (2 hours)

Introduction to Photo-electrochemistry at semiconductor electrodes, Photoemission from metal electrodes, Electro chemical monitoring of photolytic intermediates, Electrochemiluminescence (2 hours)

Unit 4. Radio-analytical Methods

Principle of Radio analytical methods- Isotope dilution analysis (1 hour),

Radiometric titrations (1 hour)

precipitation and complex formation titrations Radiometric titrations (1 hour)

precipitation and complex formation titrations (1 hour)

Unit 5. Instrumentation

UV – Visible instrumentation- light sources, detectors (2 hours),

Infra-Red Spectroscopy- principle, instrumentation (2 hours),

Luminescence (1 hours), Nuclear Magnetic Resonance (2 hours),

Mass spectrometer with various detectors- Electron multipliers, Faraday cup, Photomultiplier conversion dynode, Array detectors (2 hours),

Atomic absorption spectrometry (1 hour),

Flame photometry-principles and applications (2 hours).

Prescribed Books

- (1) D. A. Skoog, F. J. Holler and T. A. Nieman, Principles of Instrumental Analysis, 7th Ed., Saunders College publishing 2017.

- (2) D. A. Skoog, D. M. West and F. J. Holler, Fundamentals of Analytical Chemistry, Saunders College Publication, New York - 9th Ed., 2013.
- (3) G. D. Christian, Analytical Chemistry, 7th Ed. John - Wiley & Sons 2013.

Reference Books:

- (1) Vogel's Text book of Quantitative Inorganic Analysis, 6th Ed., Pearson, 2009.
- (2) Joseph Wang, Analytical Electrochemistry, 3rd Ed., Wiley VCH, 2006.
- (3) P. T. Kissinger and W. R. Heineman, Laboratory Techniques in Electro Analytical Chemistry, 2nd Ed., Marcel Dekker Inc. New York 2016.

Semester III has one Discipline Specific Elective. Students are free to opt any one from the following list.

Discipline Specific Elective I

| Semester | Course Category | Course Name | Course Code | L | T | P | C |
|-----------------|------------------------|---|--------------------|----------|----------|----------|----------|
| III | DSE | Theoretical and Physical aspects of Organic Reactions | MCH2235 | 4 | 0 | 0 | 4 |
| | | Supramolecular chemistry and modern crystal engineering | MCH2236 | 4 | 0 | 0 | 4 |
| | | Computational Chemistry | MCH2237 | 4 | 0 | 0 | 4 |

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|---|---|---|---|---|
| DSE | MCH2235 | Theoretical and Physical aspects of Organic Reactions | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Explain bonding and reactions in terms of orbital description. (B.L. 2) | | | | | |
| CLO2 | Illustrate effect of substituents in organic reactions outcome. (B.L. 2) | | | | | |
| CLO3 | Plan the reactions product outcome in the light of thermodynamic and kinetic pathways. (B.L. 3) | | | | | |
| CLO4 | Analyze the stereo-chemical outcomes of stereoselective and stereospecific organic reactions. (B.L. 4) | | | | | |
| CLO5 | Analyse the outcomes of various pericyclic and photochemical reactions. (B.L. 4) | | | | | |

UNIT 1: Molecular Orbital Theory

The Atomic Orbitals of a Hydrogen Atom; Molecules made from Hydrogen Atoms-The H_2 Molecule, The H_3 Molecule, The H_4 'Molecule'; C—H and C—C Bonds-The Atomic Orbitals of a Carbon Atom, Methane, Methylene, Hybridisation. (3 hours)

C—C σ Bonds and π Bonds: Ethane, C=C π Bonds: Ethylene; Conjugation—Huckel Theory-The Allyl System, Butadiene, Longer Conjugated Systems, Aromaticity, Aromatic Systems, Antiaromatic Systems, The Cyclopentadienyl Anion and Cation, Homoaromaticity, Spiro Conjugation. (3 hours)

Strained σ Bonds—Cyclopropanes and Cyclobutanes, Cyclopropanes, Cyclobutanes, Heteronuclear Bonds, C—M, C—X and C=O - Atomic orbital energies and electronegativity, C—X σ Bonds, C—M σ Bonds, C=O π Bonds, Heterocyclic Aromatic Systems; The Tau Bond Model. (3 hours)

Spectroscopic Methods - Ultraviolet Spectroscopy, Photoelectron Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Electron Spin Resonance Spectroscopy. (3 hours)

UNIT 2: The Structure of Organic Molecules

The Effects of π Conjugation - A Notation for Substituents, The Effect of Substituents on the Stability of Alkenes. (2 hours)

The Effect of Substituents on the Stability of Carbocations, The Effect of Substituents on the Stability of Carbanions. (2 hours)

The Effect of Substituents on the Stability of Radicals, Energy-Raising Conjugation; σ Conjugation—Hyperconjugation - C—H and C—C Hyperconjugation, C—M Hyperconjugation, Negative Hyperconjugation. (3 hours)

The Configurations and Conformations of Molecules - Restricted Rotation in π -Conjugated Systems, Preferred Conformations from Conjugation in the σ Framework. (3 hours)

Other Noncovalent Interactions - The Hydrogen Bond, Hypervalency, Polar Interactions, and van der Waals and other Weak Interactions. (2 hours)

UNIT 3: Chemical Reactions & Ionic Reactions—Reactivity

Chemical Reactions-How Far and How Fast: Factors Affecting the Position of an Equilibrium, The Principle of Hard and Soft Acids and Bases (HSAB), Transition Structures, The Perturbation Theory of Reactivity, The Salem-Klopman Equation, Hard and Soft Nucleophiles and Electrophiles, Other Factors Affecting Chemical Reactivity. (4 hours)

Ionic Reactions—Reactivity: Single Electron Transfer (SET) in Ionic Reactions; Nucleophilicity - Heteroatom Nucleophiles, Solvent Effects, Alkene Nucleophiles, The α -Effect; Ambident Nucleophiles - Thiocyanate Ion, Cyanide Ion and Nitrite Ion (and the Nitronium Cation), Enolate Ions, Allyl Anions, Aromatic Electrophilic Substitution. (4 hours)

Electrophilicity - Trigonal Electrophiles, Tetrahedral Electrophiles, Hard and Soft Electrophiles; Ambident Electrophiles - Aromatic Electrophiles, Aliphatic Electrophiles; Carbenes - Nucleophilic Carbenes, Electrophilic Carbenes, Aromatic Carbenes. (4 hours)

UNIT 4: Ionic Reactions—Stereochemistry

The Stereochemistry of the Fundamental Organic Reactions - Substitution at a Saturated Carbon, Elimination Reactions, Nucleophilic and Electrophilic Attack on a π Bond, The Stereochemistry of Substitution at Trigonal Carbon. (4 hours)

Diastereoselectivity - Nucleophilic Attack on a Double Bond with Diastereotopic Faces, Nucleophilic and Electrophilic Attack on Cycloalkenes. (4 hours)

Electrophilic Attack on Open-Chain Double Bonds with Diastereotopic Faces, Diastereoselective Nucleophilic and Electrophilic Attack on Double Bonds Free of Steric Effects. (4 hours)

UNIT 5: Radical Reactions & Photochemical Reactions

Radical Reactions: Nucleophilic and Electrophilic Radicals; The Abstraction of Hydrogen and Halogen Atoms - The Effect of the Structure of the Radical, The Effect of the Structure of the Hydrogen or Halogen Source. (2 hours)

The Addition of Radicals to π Bonds - Attack on Substituted Alkenes, Attack on Substituted Aromatic Rings; Synthetic Applications of the Chemoselectivity of Radicals; Stereochemistry in some Radical Reactions. (2 hours)

Ambident Radicals - Neutral Ambident Radicals, Charged Ambident Radicals, Radical Coupling. (2 hours)

Photochemical Reactions: Photochemical Reactions in General; Photochemical Ionic Reactions - Aromatic Nucleophilic Substitution, Aromatic Electrophilic Substitution, Aromatic Side-Chain Reactivity. (2 hours)

Photochemical Pericyclic Reactions and Related Stepwise Reactions, The Photochemical Woodward-Hoffmann Rule, Regioselectivity of Photocycloadditions. (2 hours)

Other Kinds of Selectivity in Pericyclic and Related Photochemical Reactions; Photochemically Induced Radical Reactions, Chemiluminescence. (2 hours)

Prescribed Books:

- (1) Ian Fleming, Molecular Orbitals and Organic Chemical Reactions, Student Edition, Wiley, 2009.
- (2) J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic chemistry, Oxford University Press, Sec. Ed. 2012.
- (3) Modern Physical Organic Chemistry, E. V. Anslyn and D. A. Dougherty, University Science Publishers, 2004, ISBN: 1-891389-31-9

Reference Books:

- (1) Ian Fleming, Molecular Orbitals and Organic Chemical Reactions, Reference Edition, Wiley, 2009.
- (2) L. Kürti and B. Czakó, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier, 2005, ISBN: 0-12-429785-4

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|--|---|---|---|---|
| DSE | MCH2236 | Supramolecular Chemistry and Modern Crystal Engineering | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Gain the knowledge fundamental basis of intermolecular interactions. | | | | | |
| CLO2 | Capable to explain how the non-covalent interactions can be exploited to form diverse supramolecular assemblies ranging from small molecules, soft gels and hard extended inorganic solids. | | | | | |
| CLO3 | Capable to analyse research-led overview of the current state-of-the-art in supramolecular systems. | | | | | |
| CLO4 | Acquire the knowledge of wider aspects of chemistry and functional materials accessible through combination. | | | | | |
| CLO5 | Apply the knowledge of supramolecular chemistry to construct molecular device for catalysis. | | | | | |

Unit 1: Supramolecular Chemistry

Definition of Supramolecular Chemistry, Host–Guest Chemistry, Classification of Supramolecular Host–Guest Compounds, Receptors, (2 hours)

Coordination and the Lock and Key Analogy, Definition and Measurement of Binding Constants, Cooperativity and the Chelate Effect, (2 hours)

Hydrogen Bonding, Cation– π Interactions, Anion– π Interactions, π – π Interactions, (2 hours)

Van der Waals Forces and Crystal Close Packing, Closed Shell Interactions, (2 hours)

Hydrophobic and Solvation Effects, Designing of Host, (2 hours)

The Crown Ethers, Lariat Ethers and Podands, Cryptands and Spherands, (2 hours)

Nomenclature of Cation-Binding Macrocycles, Calixarenes and Siderophores. (2 hours)

Unit 2: Introduction to Crystal Engineering

Definition of Crystal Engineering, (1 hour)

Special Role of Hydrogen Bonding, Etter's Rules, (2 hours)

Crystal Engineering Design Strategies, (1 hour)

Importance and types of Polymorphism; Scope, Nomenclature and Design Principle of Co-crystals, (1 hour)

Explanation of Tectons and Synthons, (1 hour)

Hydrogen Bonds to Rings, Halogens, Cyanometallates, CO Ligands and Metals and Metal Hydrides, (2 hours)

Edge-to-Face and Face-to-Face Interactions in Aromatic Rings, Halogen Bonding and Other Interactions. (2 hours)

Unit 3: Crystal Nucleation and Growth and Molecular Guests

Theory of Crystal Nucleation and Growth, Crystal Growth at Air–Liquid Interfaces, Chirality Induction (2 hours)

The Adam Effect, Hourglass Inclusions, Epitaxy (2 hours)

Engineering Crystals, Mechanochemistry and Topochemistry, Dendrimer Host–Guest Chemistry. (2 hours)

General Considerations of Molecular Guests in solution, Building Blocks, Dynamics of Guest Exchange in Cavities, (2 hours)

Inclusion Chemistry of Cyclodextrins, Cyclophane Nomenclature, Guest Inclusion by Hydrogen Bonding, (2 hours)

Definitions and Synthesis of Covalent Cavities, Carcerands and Hemicarcerands, Giant Covalent Cavities. (2 hours)

Unit 4: Network Solids and Self-Assembly

Concepts and Classification of Network Solids, Network Topology and Porosity, (2 hours)

Synthesis, Composition and Structure of Zeolites, Layered Solids and Intercalates, (2 hours)

Hoffman Inclusion Compounds and Werner Clathrates, Coordination Clusters, 0D, 1D, 2D and 3D Structures, (1 hour)

Interpenetrated Structures, Porous and Cavity-Containing Structures. (1 hour)

Concepts and Classification of Self-Assembly, Protein Self-Assembly, Foldamers, Strict Self-Assembly, Double Mutant Cycles – Quantifying Weak Interactions, (2 hours)

A Supramolecular Cube, Tennis Balls and Softballs (2 hours)

Self-Complementary Assemblies, Heterodimeric Capsules, Rosettes, Rotaxanes and Catenanes Involving π - π Stacking Interactions, Helicates, (2 hours)

Topology of Knots, Trefoil Knots, Other Knots. (2 hours)

Unit 5: Molecular Device and Supramolecular Catalysis

Introduction of Molecular Devices, when is a Device Supramolecular? Molecular Electronic Devices, Wires, (2 hours)

Rectifiers and Switches, Photophysical Fundamentals, (2 hours)

Mechanisms of Energy and Electron Transfer, (2 hours)

Enzyme Modelling Using an Artificial Host Framework, (2 hours)

Abiotic Supramolecular Catalysis, Dynamic Combinatorial Libraries, Self-Replicating Systems. (2 hours)

Prescribed Books

(1) W. Steed, Jerry L. Atwood, Supramolecular Chemistry, Second Edition, 2009. ISBN: 9780470512333, DOI: 10.1002/9780470740880.

(2) Jean-Marie Lehn, Wiley-VCH; 1st edition, 1995, Supramolecular Chemistry: Concepts and Perspectives, Germany. ISBN-13: 978-3527293117.

(3) Peter J. Cragg, Supramolecular Chemistry, Springer Nature, Switzerland, 2014. ISBN 978-90-481-2581-4. DOI: <https://doi.org/10.1007/978-90-481-2582-1>

Reference Books

(1) J. L. Atwood, and J. W. Steed, Encyclopedia of Supramolecular Chemistry, Marcel Dekker, New York, NY, USA, 2004.

(2) E. V. Anslyn, and D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books: Sausalito, California, USA, 2006.

- (3) P. J. Cragg, Practical Supramolecular Chemistry, John Wiley & Sons, Ltd., Chichester, UK, 2006.
- (4) G. R. Desiraju, The Crystal as a Supramolecular Entity, John Wiley & Sons, Ltd., Chichester, UK, 1996.
- (5) J.-M. Lehn, Supramolecular Chemistry, VCH, Weinheim, Germany, 1995.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|-------------------------|---|---|---|---|
| DSE | MCH2237 | Computational Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | To develop the knowledge of computational chemistry | | | | | |
| CLO2 | To construct different formalism for solving chemical problems computationally | | | | | |
| CLO3 | To develop the understanding of density functional theory (DFT) | | | | | |
| CLO4 | To implement DFT in solving electronic structure problems | | | | | |
| CLO5 | To develop and implement Molecular mechanisms and Monte Carlo simulations for solving chemical problems | | | | | |

Unit 1: Introduction to Computational Chemistry

Introduction and scope of computational chemistry (1 hour),

Potential energy surface, conformational search, global minimum, local minima, saddle points (2 hours).

[3 lectures]

Unit 2: Ab-initio methods

A review of Hartree-Fock method, self-consistent field (SCF) procedure. Roothan concept basis functions (3 hours)

Basis sets and its classification: Slater type and Gaussian type basis sets, minimal basis set, Pople basis sets (4 hours)

Post Hartree-Fock methods - introduction to Møller Plesset perturbation theory, configuration interaction, coupled cluster and semi empirical methods (5 hours).

[12 lectures]

Unit 3: Introduction to Density Functional Theory (DFT) methods

Idea of functional, Functional derivatives, Electron density (2 hours),

Thomas Fermi model, Hohenberg-Kohn theorems (3 hours),

Approximations for exchange-correlation: Local density approximation (LDA) and local spin density approximation (LSDA), Gradient expansion and generalized gradient approximation (GGA), Hybrid functional and meta-GGA approaches (6 hours)

Self-interaction corrections (SIC). Kohn-Sham formulation: Plane waves and pseudo potentials, Janak's theorem, Ionization potential theorem, Self-consistent field (SCF) methods (6 hours)

Understanding why LDA works, Consequence of discontinuous change in chemical potential for exchange-correlation, Strengths and weaknesses of DFT (4 hours).

[21 lectures]

Unit 4: Electronic Structure with DFT

Free electron theory, Band theory of solids (2 hour),

Tight-binding method, Band structure, Density of states (3 hours)

Interpretation of Kohn-Sham eigenvalues in relation with ionization potential (2 hours)

Fermi surface and band gap (2 hour).

[9 lectures]

Unit 5: Molecular Dynamics and Monte Carlo simulation

Equations of motion, Integration algorithms, Constraint dynamics (2 hours),

Periodic Boundary Condition and Minimum Image Convention, Structural and Dynamical Properties from MD (4 hours),

Markov Chains, Metropolis Algorithm, Structural Properties from MC (4 hours),

Brownian motion, Langevin Equation, Diffusion Constant and Velocity auto-correlations (5 hours)

[15 lectures]

Prescribed Books

- (1) Richard M. Martin, Electronic Structure: Basic Theory and Practical Methods, (Cambridge University Press, (2004)
- (2) D. Frenkel and B. Smit, Understanding Molecular Simulations: From Algorithms Applications, Second Edition, Academic Press, (2002)
- (3) Robert G. Parr and Weitao Yang, Density Functional Theory of Atoms and Molecules, (Oxford University Press, 1994).
- (4) Andrew R. Leach Molecular Modelling Principles and applications. II ed. Prentice Hall (2001)

(5) June Gunn Lee, Computational Materials Science: An Introduction, (CRC Press 2011)

References Books

- (1) David S. Sholl and Janice A. Steckel, Density Functional Theory: A Practical Introduction (John Wiley and Sons, 2009).
- (2) M. E. Tuckerman, Statistical Mechanics: Theory and Molecular Simulations, Oxford University Press, (2010)

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|-----------------------------------|---|---|---|---|
| CP | MCH2238 | Practical Computational Chemistry | 0 | 0 | 4 | 2 |
| Course Learning Outcome | | | | | | |
| CLO1 | To plan and carry out computational work using various tools | | | | | |
| CLO2 | To analyse computational data using various tools | | | | | |
| CLO3 | Use of DFT and MD simulations for understanding chemical reactions | | | | | |

Introduction to Gaussian calculations, carrying of conformational analysis of small molecules, Vibrational spectra, NMR spectra and TDDFT calculations, Modelling chemical reactions including transition state calculations., 2D potential energy surface generation for two torsion angles.

Building macromolecules, extracting crystal structure/NMR coordinates and generating models for MD simulations. RESP charge calculation. Energy minimization during MD simulations- Steepest descent and conjugate gradient methods. Gas phase MD simulations. MD simulations in implicit solvent. MD simulations in explicit solvents.

References:

- (1) Computational Chemistry and Molecular Modeling Principles and Applications by K. I. Ramachandran · G. Deepa, K. Namboori, 2008 Springer-Verlag Berlin Heidelberg, ISBN-13 978-3-540-77302-3.
- (2) COMPUTATIONAL CHEMISTRY Introduction to the Theory and Applications of Molecular and Quantum Mechanics Errol Lewars, 2004 Kluwer Academic Publishers New York, Boston, Dordrecht, London, Moscow, ISBN: 1-4020-7285
- (3) Understanding Molecular simulations From algorithms to applications by Frenkel D and Berend S, 2002 Academic Press New York
- (4) Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems. David C. Young Copyright (2001) John Wiley & Sons, Inc.

| Course category | Course Code | Course Name | L | T | P | C |
|------------------------|--------------------|--------------------|----------|----------|----------|----------|
| P | MCHR2239 | Project I | 0 | 0 | 4 | 2 |

This is the first part of MSc project which is to be carried out in the university. Under the guidance of their chosen MSc supervisor students would learn following Units. Per week the students have to spend minimum 4 hours in lab or reading as instructed by their MSc supervisor.

Unit 1: Introduction to research and independent learning

Unit 2: Understanding Research Methods, Research skills, time management and Project development

Unit 3: Drafting research proposals, Plagiarism test and Presentation

At the end of the semester, a presentation in the form of a research proposal has to be presented in front of the committee. The committee for this purpose will be constituted by the Head of the department with consultation with student's supervisor consisting of not less than two internal faculty members.

SEMESTER IV

Students in semester IV have to take two DSE and one OE. Students are free to opt any courses from following list:

Discipline Specific Elective II

| Semester | Course Category | Course Name | Course Code | L | T | P | C |
|----------|-----------------|--------------------------------------|-------------|---|---|---|---|
| IV | DSE | Organic Chemistry of Natural Product | MCH2241 | 4 | 0 | 0 | 4 |
| | | Photo-Inorganic Chemistry | MCH2242 | | | | |
| | | Solid State: Theory & Applications | MCH2243 | | | | |

Discipline Specific Elective III

| Semester | Course Category | Course Name | Course Code | L | T | P | C |
|----------|-----------------|---|-------------|---|---|---|---|
| IV | DSE | Polymer Chemistry | MCH2244 | 4 | 0 | 0 | 4 |
| | | Chemistry of Nanomaterials and their Applications | MCH2245 | | | | |

List of Open Elective (OE)

Open elective Courses offered by the Department of Chemistry is open to the students of all the department of the university. The courses are interdisciplinary in nature.

| Semester | Course Name | Course Code | L | T | P | C |
|----------|---------------------------|-------------|---|---|---|---|
| IV | Pharmaceuticals Chemistry | MCH2246 | 4 | 0 | 0 | 4 |
| | Environmental Chemistry | MCH2247 | | | | |

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|---------------------------------------|---|---|---|---|
| DSE | MCH2241 | Organic Chemistry of Natural Products | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Summarize the biosynthetic pathways of natural products. (B.L. 2) | | | | | |
| CLO2 | Compare the properties of Terpenes, Steroids and Alkaloids. (B.L.2) | | | | | |
| CLO3 | Apply knowledge of principles of natural products towards syntheses of natural products. (B.L.3) | | | | | |
| CLO4 | Examine the natural products involved in plant defence system. (B.L.4) | | | | | |
| CLO5 | Critically analyse and interpret the data from current literature concerning natural products (B.L.4) | | | | | |

Unit 1: Introduction to Natural Products

Methods in Natural product chemistry: Techniques used in isolation and determination of structures of different types of plant secondary metabolites. (6 hours)

Biosynthesis: A brief introduction to acetate malonate, acetate mevalonate and shikimic acid pathways. (6 hours)

Unit 2: Terpenes & Steroids, and Alkaloids

Terpenes and Steroids: structure elucidation of citral, photochemistry of santonin: synthesis of longifolene: total synthesis of steroid hormones. Synthesis of Prostaglandins (PGF_{2α}). (4 hours)

Alkaloids: Biosynthesis of opium alkaloids: Stereochemistry and rearrangements of morphine: determination of structure of strychnine and eudistomin K: stereochemistry and total synthesis of reserpine: stereochemistry and synthesis of quinine: photochemistry of Colchicine (8 hours)

Unit 3: Antibiotics

Oxygen Heterocyclic Compounds: Structure elucidation of flavonoids with a suitable example (use of colour reactions, UV, MS, ¹³C & ¹H NMR): total synthesis of Gilvocarcin M&V: Determination of structure of scandenin by spectral methods. (6 hours)

Corrins: Synthesis of cyanocobalamin. (3 hourss)

Antibiotics: Reactions & synthesis of penicillin, total synthesis of anti-cancer antibiotics such as daunorubicin. (3 hours)

Unit 4: Chemical Ecology

An introductory study: chemistry of insects with particular reference to chemical defence mechanisms. (6 hours)

pheromones - Plant defence chemicals - Allelo - chemicals and Phytoalexins (examples and their use in agriculture). (6 hours)

Unit 5: Problem-Solving sessions

Critical analysis and interpretation of data from current literature concerning natural products. (12 hours)

Prescribed Books:

- (1) N. R. Krishnaswamy, Chemistry of Natural Products – A Unified Approach, University Press, Hyderabad, 1999.
- (2) K. Nakanishi et al (Editors) Natural Products, Vols 1, 2 and 3, Academic press 1974, 1975 and 1983.
- (3) K. C. Nicolaou and E. J. Sorensen, Classics in Total Syntheses, VCH, 1996.
- (4) J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne ,Natural Products, Addison Wesley Longman Limited, 1994.
- (5) J. Apsimon (Editor), Total synthesis of Natural products, Vols I, V and VI Academic Press, 1973, 1983 and 1984.

Reference Books:

- (1) Coffey (Editor), Rodd's Chemistry of Carbon Compounds, Vols. 2 C, D, and E with supplements and volumes 4E, G and H, Elsevier 1974 to1985.
- (2) Barton Oilis (Editor), Comprehensive Organic Chemistry Ed. by Barton Oilis, Vol. 5, Biological compounds, Pergamon press, 1979.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|---------------------------|---|---|---|---|
| DSE-2 | MCH2242 | Photo-Inorganic Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Define the underlying principles of photo chemistry | | | | | |
| CLO2 | Make use of the photochemistry laws to explain the Photochemical Properties of Transition Metal Complexes | | | | | |
| CLO3 | Distinguish between the different mechanisms for the colour of transition metal complexes. | | | | | |
| CLO4 | Apply the basic understanding of photochemistry in different applied field of chemistry | | | | | |
| CLO5 | Explain the Photochemical Reactions on Solid Surface | | | | | |

Unit I: Principles of Photochemistry

Absorption, excitation, photochemical laws, quantum yield. Absorption and emission for complexes with different ground state /excited state for ML_6 complexes. Potential energy function and energy levels for ML_6 complexes. (6 hours)

Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra. (3 hours) Frank-Codon principle, photochemical stages – primary and secondary processes. Jablonski diagram for photochemical process. (3 hours)

Unit 2: Photochemical Properties of Transition Metal Complexes

Photo physical process, photochemical process, Photo substitution reactions,(4 hours) photo-redox reactions, Photo rearrangement reaction. (4 hours)

Prompt and Delayed Photochemical reactions, Photolysis rules and ligand field theory. (4 hours)

Unit 3: Charge Transfer Photochemistry

Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level scheme for charge transfer excitations. (4 hours)

Types of reactions observed by charge transfer metal complexes. (6 hours)

Unit 4: Ligand Field Photo chemistry of Transition Metal Complexes

Photochemistry Cr(III) of complexes: Photo-substitutions, properties of ligand field excited states, Photo aquation reactions, photolysis rule , photo isomerization , photo racemization, photoanation reactions, sensitizer, energy transfer process. (5 hours)

Mechanism of photosensitization, photo reactive excited state. The Doublet hypothesis, Role of quartet excited states. (4 hours)

Photochemistry of Co(III) complexes : Introduction, energy level diagram, Photo aquations in Co(III) amine, Co(III) cyanide complexes, Fe(II) low spin complexes, Ru(II) ammine derivative complexes, Photo redox properties of Ce(III) and Ce(IV) complexes, photochemistry of Cu(II) (1,3 diketone) complexes (5 hours)

Unit 5: Photochemical Reactions on Solid Surface

Introduction, photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels. (3 hours)

Examples of photo catalytic metal/mixed metal oxides and their applications, semiconductor supported metal oxides for photolysis of water, Decomposition of organic pollutants, experimental setup, end product of organic products, carbon dioxide reduction, nitrogen fixations, solar energy conversion and its storage. (7 hours)

Chemiluminescence's in coordination complexes, Thexi state and Franck Condon state.

(3 hours)

Prescribed Books

1. D.M Roundhill, Photochemistry and Photophysics of Metal Complexes, 1994, Springer
2. Adamson, A.W and Fleischauer, P.D (1975): Concepts of Inorganic Photochemistry, Wiley, New York.
- 3.K.K Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2018, NEW AGE INTERNATIONAL (P) LIMITED, PUBLISHERS.

3. Ferraudi , G.J (1988): Elements of Inorganic Photochemistry, Wiley, New York.

Reference Books

1. Lever, A. B. P (1984): Inorganic Electronic Spectroscopy, Elsevier Science.
2. Veera Reddy, K (1998): Symmetry and Spectroscopy of Molecules, New Age International.
3. V. Balzani and V. Carasiti, Photochemistry of Co-ordination compounds, Academic Press, 1970.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|------------------------------------|---|---|---|---|
| DSE | MCH2243 | Solid State: Theory & Applications | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | To define crystals symmetries and find crystal structures from XRD pattern of solids. | | | | | |
| CLO2 | To build mathematical formulation of vibrational mode in solids, Heat capacity and thermal properties | | | | | |
| CLO3 | To demonstrate various defects present in the solids and their properties | | | | | |
| CLO4 | To develop the understanding of free electron gas theory and band structures of solids | | | | | |
| CLO5 | To explain magnetic properties of various solids and superconductivity | | | | | |

Unit 1: Crystals and Solid state Reactions

Brief introduction to crystal and Concept of reciprocal space (3 hours),

Thermodynamics of solid, crystallization kinetics, synthetic strategy (2 hours)

[5 Lectures]

Unit 2: Crystal Vibrations and Thermal properties

Vibrations of Crystals with Monatomic Basis (1 hours),

Group Velocity, Long Wavelength Limit (1 hours),

Derivation of Force Constants from Experiment, Quantization of Elastic Waves, Phonon Momentum (3 hours),

Inelastic Scattering by Phonons, Phonon Heat Capacity, Planck Distribution (3 hours),

Normal Mode, Density of States in One Dimension and Three Dimensions, Debye T^3 Law, Einstein Model, Thermal Conductivity (3 hours)

[11 Lectures]

Unit 3: Imperfections in solids

Frenkel and Schottky defects (1 hour),

Defects by non-stoichiometry; electrical conductivity of ionic crystals (2 hours);

Classifications of dislocations; role of dislocations in plastic deformation and crystal growth;

Colour centers and photoconductivity (3 hours);

Luminescence and phosphors (1 hour);

[7 Lectures]

Unit 4: Free Electron Gas and Band Theory

Free electron gas model of metals (2 hours),

Free electron gas in a one-dimensional and three dimensional box (1 hour),

Bloch theorem, Kronig-Penny model, tight binding approximation (3 hours),

Band theory of insulators and semiconductors (2 hours),

Intrinsic semiconductors, extrinsic semiconductors, doped semiconductors (3 hours)

[11 Lectures]

Unit 5: Magnetic properties of solids and Superconductivity

Origin of magnetism; Diamagnetism: quantum theory of atomic diamagnetism; Landau diamagnetism (qualitative discussion) (3 hours);

Paramagnetism: classical and quantum theory of para-magnetism (2 hours);

Case of rare-earth and iron-group ions; quenching of orbital angular momentum (2 hours);

Van-Vleck Paramagnetism and Pauli Paramagnetism (1 hour)

Ferromagnetism: Curie-Weiss law, temperature dependence of saturated magnetization (2 hours),

Heisenberg's exchange interaction, Ferromagnetic domains - calculation of wall thickness and energy (2 hours);

Ferrimagnetism and antiferromagnetism (1 hours).

Superconductivity: Introduction of the phenomenon (1 hours),

London's equations and penetration depth, quantized flux, coherence length (3 hours).

Ginzburg-Landau theory (2 hours),

Variation of the order parameter and the energy gap with magnetic field (1 hour),

Isotope effect; Energy gap and its measurement (2 hours);

Electron-phonon interaction and cooper pairs (2 hours),

Brief discussion of the B.C.S. theory (2 hours).

[26 Lectures]

Prescribed Books

- (1) A. R. West, Solid State Chemistry and its Applications, (2001) John Wiley and Sons, Singapore.
- (2) Neil W. Ashcroft, N David Mermin, Solid State Physics Paperback – 1 December (2003)
- (3) Elaine A. Moore, Lesley E. Smart, Solid State Chemistry: An Introduction (5th Edition) (2011)

References

- (1) Stephen Blundell, Magnetism in Condensed Matter (Oxford Master Series in Physics) (Oxford University Press: 1st Edition) (2002)
- (2) Assa Auerbach, Interacting Electrons and Quantum Magnetism (Springer; Softcover reprint of the original 3st ed. 2001 edition)
- (3) C. Kittel, Introduction to Solid State Physics, John Wiley & Sons, Inc., New York, Chichester (2006)

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|---|-------------------|---|---|---|---|
| DSE | MCH2244 | Polymer Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | To classify different ways of synthesising macromolecules | | | | | |
| CLO2 | To analyse the structure of macromolecules | | | | | |
| CLO3 | To develop the theory of polymers | | | | | |
| CLO4 | To identify different alloys and composite of polymer | | | | | |
| CLO5 | To examine polymer degradation and stabilisation | | | | | |

Unit 1: Synthesis of Macromolecules – Molecular Mass of Polymers

Concept of macromolecules, Classification, Functionality and principles of polymerization, Different polymerization techniques, Kinetic chain length, gelation, Branching and crosslinking (2 hours)

Step-growth polymerization, Carothers Equation, Ring opening polymerization, Plasma polymerization, Copolymer-Copolymer equation, Monomer reactivity Ratio, Q-e scheme (3 hours)

Molecular mass of Polymers: Molecular mass distribution, Distribution curve, Polydispersity index, Different types of Average Molecular mass determination - Absolute and relative methods (3 hours)

Colligative properties: ebullioscopy, Cryoscopy, endgroup analysis, Membrane Osmometry, Vapor phase Osmometry, Light scattering, Ultracentrifugation. (2 hours)

Solution viscosity - Intrinsic viscosity, Determination of viscosity average molecular weight, Mark-Houwink equation (2 hours)

Fractionation of polymers- Gel permeation chromatography (GPC), Relation of chromatogram shape and MWD (2 hours)

[14 Lectures]

Unit 2: Investigation of Polymers – Structure and configuration

Chiral polymers, tacticity, conformation of single molecules, freely jointed chain, random flight model, and Average chain dimension. End to end distance (2 hours)

Restriction due to bond angles, Conformation in crystal and micro conformation. Secondary bond forces, chain configuration, (2 hours)

Basic determination of polymer properties: Ring structure and its significance, chain flexibility and factors affecting it. (2 hours)

Elastomers, fibers and plastics- Property requirements and application. (2 hours)

Glass transition temperature and crystalline melting point

[10 Lectures]

Unit 3: Theory of Polymer Solution: Ideal and Non-ideal Solution

Thermodynamics of polymer solution- Entropy, enthalpy, and free energy of mixing (3 hours)

Lattice model-solubility parameter, free volume theory, Excluded volume (2 hours)

Flory-Huggins Theory, Flory-Krigbaum theory, Huggins and Kraemer equation (2 hours)

Phase equilibria in polymeric systems. Critical solution temperature, LCST and UCST behavior. (3 hours)

Experimental results in binary systems involving polymer blends. (1 hours)

[11 Lectures]

Unit 4: Polymer blend alloys and composites

Importance of polymer blending-Blending techniques. Miscible and immiscible blends, Miscibility through specific interactions. (3 hours)

Polymer alloys, Phase diagram of polymers, polymer systems. (2 hours)

Blend morphology, characteristics of FTIR, Fluorescent spectroscopy, microscopy, Compatibilization of miscible blends. (2 hours)

Addition of graft or copolymers. Types of compatibilities: in situ formed, separately added polymers. (2 hours)

Polymer composites: Role of fiber and matrix in improving composite properties bonding between fiber and matrix. Critical fiber length in short fiber composites. Role of composites in aerospace application. (2 hours)

Composite fabrication techniques: Open model process, vacuum bag molding, centrifugal casting and pultrusion. Closed model process - matched die molding, thermoforming injection molding. (3 hours)

[14 lectures]

Unit 5: Polymer degradation and stabilization

Chemical degradation, physical degradation, ageing, crazing, degradation by microorganisms, (3 hours)

Biodegradable polymers, Mechanism of degradation, secondary chain reaction, Self-reaction, depolymerisation. (3 hours)

Metal catalyzed degradation, Thermal oxidation, Photo oxidation, Mechanical degradation, Degradation by ionizing radiation, ozone attack. (3 hours)

Degradation of special polymers: Polyolefin, PVC, PS, PMMA. (2 hours)

[11 Lectures]

Prescribed Books

- (1) R. J. Young, Introduction to polymer science, CRC Press, 3rd edition, 2011
- (2) G. Odian, Principles of polymerization, Wiley, 4th edition 2004.
- (3) F. W. Billmeyer, Text book of polymer science, Wiley, 3rd edition 2001.
- (4) K. K. Chawla, Composite materials, Springer 2011.

References Books:

- (1) D. R. Paul and Newman, Polymer blends, Vol 1 and 2, Academic, 1st edition, 1978. Digitalized, Oct 2009.
- (2) O. Olabisi, Polymer-polymer miscibility, Academic, 2000.
- (3) F. R. Jones, Handbook of polymer fiber composites, Longman, 1st edition, 2001

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|--|---|---|---|---|
| DSE | MCH2245 | Chemistry of Nanomaterials and their Application | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Obtain the knowledge about different advanced materials. | | | | | |
| CLO2 | Evaluate the properties of new materials and their analysis. | | | | | |
| CLO3 | Analyse the structure and bonding of new materials. | | | | | |
| CLO4 | Get the knowledge of development and application of advanced materials and their associated processing and manufacturing technologies. | | | | | |
| CLO5 | Gain an idea of assembly of organic, inorganic, coordination and biological molecules and higher-level building units. | | | | | |

Unit 1: Introduction to nanomaterials

Introduction of nanomaterials, Classification and nomenclature of nanomaterials, (2 hours)
 Characteristics of Nanomaterials: Nucleation and growth of nano systems, self-assembly, functional nanomaterials, (2 hours)

Crystal structure of materials, packing fraction, basics of solid-state chemistry, specific surface energy and surface stress and effect on the lattice parameter, (2 hours)

Size and shape dependent optical, emission, electronic, transport, photonic, refractive index, dielectric, mechanical, magnetic, (2 hours)

Non-linear optical properties; transition metal sols, origin of Plasmon band, Mie theory. (2 hours)

Unit 2: Transition Metal Di-Chalcogenides (TMDs)

2D TMDs: Impact, Synthesis, and Properties; Scientific Impact of 2D TMDs, 1D TMDs: Achievements and Features; (2 hours)

Synthesis and Fabrication Challenges: Top-down and Bottom-up; (2 hours)

Physical Properties of 1D TMDs, Role of Edges and Defects, Optical and Electronic Effects, (2 hours)

Analytical Tools for Characterizing and Manipulating TMDs, (2 hours)

In Situ Probes to Manipulate TMDs, Research Areas and Opportunities: Catalysis, Heterostructure and Optoelectronic and Neuromorphic Devices. (4 hours)

Unit 3: MXenes and their application

Introduction of MXenes, Methods to obtain mxenes. (2 hours)

Urea glass route, Chemical vapor deposition, Molten salt etching, Hydrothermal synthesis in an aqueous NaOH solution, Electrochemical synthesis at room temperature. (2 hours)

MXene properties: Mechanical properties, electronic properties, Magnetic properties, Optical properties, (2 hours)

Applications: Energy storage and conversion, MXenes for antenna applications, (2 hours)

Application to environmental challenges, biological applications, Sensor activity, etc. (4 hours)

Unit 4: Graphene and its analogues

Introduction to graphene, History of graphene, (2 hours)

Synthesis of graphene: Mechanical Exfoliation, Liquid Phase Exfoliation, Unzipping of Carbon Nanotube (2 hours)

Discharge Method, Chemical Vapor Deposition (CVD), Epitaxial Growth of Graphene in Silicon Carbide (SiC), Oxidation-Reduction. (2 hours)

Applications: Lithium-Ion Batteries, Supercapacitors, (2 hours)

Electrochemical Sensors, Transparent Electrodes, Environmental Applications, (2 hours)

Adsorption of Metal Ions, Adsorption of Gases. (2 hours)

Unit 5: Metal-Organic Frameworks (MOFs) & Covalent Organic Frameworks (COFs)

Introduction to Metal-Organic Frameworks (MOFs), Terminology of MOFs, Design of MOFs, (1 hour)

Synthetic procedure of MOF, conventional solvothermal synthesis, microwave-assisted synthesis, sonochemical synthesis, electrochemical synthesis, mechanochemical synthesis, Dry-gel Conversion MOF Synthesis; (2 hours)

Structure of MOFs: Special features of MOF structures and their difficulties; (2 hours)
Versatile applications of MOF in gas adsorption and storage, organic catalysis, drug delivery, photocatalysis, electrocatalysis, solution to environmental threats etc. (3 hours)

Introduction to Covalent Organic Frameworks (COFs), Design principles and bond formation of COFs, Linkage types of COFs, (1 hour)

Synthetic procedure of COF: Solvothermal synthesis, Microwave synthesis, sonochemical synthesis, mechanochemical synthesis, Light-induced synthesis, other methods. (3 hours)
Applications; Carbon dioxide storage, Catalysis, Supercapacitors etc. (2 hours)

Prescribed Books:

(1) Materials Science and Engineering: A First Course, V. Raghavan, 6th Edition, Prentice Hall India Learning Pvt. Ltd., 2004.

(2) Materials Science and Engineering, D. G. Rethwisch, W. Callister, 10th Edition, John Wiley & Sons Inc, 2018.

(3) Advanced 2D Materials, A. Tiwari, M. Syväjärvi, John Wiley & Sons, Ltd., Chichester, UK, 2016.

Reference Books:

(1) Introductory Nanoscience, M. Kuno, 2011, Taylor & Francis Group.

(2) Carbon Nanotubes: Synthesis, Structure, Properties, and Applications, M. S. Dresselhaus, G. Dresselhaus, P. Avouris, Springer-Verlag., 2001.

List of Open Elective (OE)

Open elective Courses offered by the Department of Chemistry is open to the students of all the department of the university. The courses are interdisciplinary in nature.

| Semester | Course Name | Course Code | L | T | P | C |
|-----------------|---------------------------|--------------------|----------|----------|----------|----------|
| Semester | Pharmaceuticals chemistry | MCH2246 | 4 | 0 | 0 | 4 |
| | Environmental Chemistry | MCH2247 | 4 | 0 | 0 | 4 |

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------------|---|--------------------------|---|---|---|---|
| DSE | MCH2246 | Pharmaceutical Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome (CLO) | | | | | | |
| CLO1 | To give a brief outline involved in the process of drug design and to understand the basic aspects related to it. | | | | | |
| CLO2 | To give an understanding of chemistry of some essential vitamins and antibiotics. | | | | | |
| CLO3 | To highlight the importance of drugs from natural products with special reference to medicinal plants of Indian and Chinese origin. | | | | | |
| CLO4 | To understand basic aspects related to polymer stability and polymer degradation in the environment. | | | | | |

Unit 1: Introduction classification of drugs based on site of action

CNS DRUGS:

Classification- CNS depressants, general CNS stimulants. (1 hour)

Analgesics- classification- narcotic and non- narcotic analgesics - characteristics
Narcotic analgesics: Site of action, mode and binding site. Mechanism of action and narcotics side-effects, withdrawal symptoms, toxicity. Exogenous opioids: Examples of narcotic analgesics- morphemes and analogue description, Mepindine and its derivatives, Methadone and its derivatives- structural activity relationships. Endogenous opioids: Enkephalins- general features- mode of action. (3 hours)

General anesthetics: Definition of anaesthesia, stages, classification, mode of action, examples.
Sedatives and Hypnotics: Definition- application- mode of action. Barbiturates mechanism of action- structural activity relationships- general synthesis- toxicity and side effects. (2 hours)

Local anaesthetics: Definition- classification, site, mode of action.
Examples: Benzoic acid derivatives and lidocaine derivatives. Structural activity relationships.
Non- narcotic analgesics: Definition, general characteristics, mode and mechanism of anti-analgesic and anti- inflammatory properties. Examples: Salicylates, *p*- Aminophenol

derivatives- structural activity relationships. Synthesis of analgesics in current use. CNS stimulants: General characteristics- site, mode and mechanism of action, structural activity relationships in Amphetamines. (3 hours)

CVS DRUGS:

Anti-coagulants: Mechanism of blood clotting- strategies in prevention of coagulation. Definition, mechanism of anti- coagulant action of Dicoumarals, structural activity relationships. (1 hour)

Anti allergic drugs: Definition- allergy, mediators of allergy- mechanism of origin of allergy- immunoglobulins. (1 hour)

Anti-Histamines: Classification- H1 Antagonists- example- mode of action-pheniramines, side effects. (1 hour)

Hydrogen antagonists- examples- mode of action. Anti- hypertensive: Hypertension definition- cause of hypertension- classification with examples - brief account of the mode of action. (2 hours)

CHEMOTHERAPEUTIC AGENTS:

Chemotherapy- definition and characteristics- distinction between chemotherapeutic agent and pharmacodynamics agent. (1 hour)

Synthetic chemotherapeutic agents: Sulphur drugs- mode of action and synthesis of currently used sulphur drugs. (1 hour)

Antibiotics- definition- characteristics. Chloramphenicol - synthesis and mode of action. Penicillins: Structural elucidation- synthesis- mode and mechanism of action- structure-activity relationships (1 hour)

Chemistry and pharmacology of streptomycin, Structure, mode of action and Pharmacology of tetracycline, gramicidin, a survey of anticancer antibiotics. (1 hour)

Vitamins-Structural elucidation, mechanism of actions, synthesis (2 hours)

Unit 2: Drug Design

The drug discovery process - conceptual back-ground - Drug receptors - drug target binding forces (3 hours)

History and development of QSAR – effect of physical properties of the drug on its action (Ferguson and related theories)- concept of lead structure & pharmacophore (4 hours)

concept of isosterism and bioisosterism- three dimensional structure (3 hours)

Aided drug design (use of PC Spartan / Hyperchem lite / PC Spartan plus software packages, to get hands on experience). (5 hours)

Unit 3: Pharmacokinetics & Pharmacodynamics

Introduction of drug absorption, bioavailability (factors effecting and dosage determination) and metabolism -Phase I & Phase II. (15 hours)

Unit 4: Dietary factors

Study of water-soluble vitamins, Chemistry and biological functions of thiamine, riboflavin, pyridoxine, pantothenic acid and folic acid. (5 hours)

Unit 5: Drugs from medicinal plants

A study of active ingredients of some well-established Indian medicinal plants; A survey of Chinese medicinal plants. (5 hours)

Prescribed Books:

- (1) Donal J Abraham, Michael Myers, (Editors) Burger's Medicinal chemistry, Drug Discovery and Development, Volume I, 8th Edition, Wiley Publishers, 2021.
- (2) Medicinal Chemistry by Ashutosh Kar, 7th Edition, New Age Publishers, 2018.
- (3) Victoria F. Roche, S. William Zito, T.L. Lemke and D.A. Williams, South Asian Edition of Foye's Principles of Medicinal Chemistry, 8th Edition, Wolters Kluwer Publishers, 2019.
- (4) I. L. Finar, Organic Chemistry Volume 2: Stereochemistry and the Chemistry Natural Products, 5th edition, Paperback, Pearson Publishers, 2002.

Reference Books:

- (1) John B. Taylor, David J. Triggle (Editors) Comprehensive Medicinal Chemistry II, Elsevier Science, 2007.
- (2) Robert K. Murray, Harper's Illustrated Biochemistry, 27th International Edition. Cbspd publishers, 2006.
- (3) Wilson and Gisvold's Textbook of Organic, Medicinal & Pharmaceutical Chemistry, 12th Ed., edited by J.N. Delgado and W. A. Remers, Lippincott-Raven Publications, 2010.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|-------------------------|---|---|---|---|
| DSE | MCH2247 | Environmental Chemistry | 4 | 0 | 0 | 4 |
| Course Learning Outcome | | | | | | |
| CLO1 | Demonstrate knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil. (BL 2) | | | | | |
| CLO2 | Recognize different types of toxic substances & responses and analyze toxicological information. (BL 2) | | | | | |
| CLO3 | To create awareness about various water purification methods, waste water treatment methods and the chemistry involved. (BL 3) | | | | | |
| CLO4 | To study the cause and effect of environmental pollution by hazardous wastes and some mitigation strategies. (BL 3) | | | | | |
| CLO5 | To explain the present energy crisis and different aspects of sustainability and to understand the role of values in addressing environmental issues. (BL 4) | | | | | |

Unit 1. Air Pollution

Air pollutants - Air quality standards, Production, fate, effects and control of gaseous pollutants (4 hours)

Oxides of carbon, nitrogen and Sulphur - Organic air pollutants (4 hours),

Photochemical reactions, photochemical smog, Greenhouse effect, Acid rain and Ozone depletion (4 hours).

Particles in the atmosphere - physical behaviour - physical and chemical processes for particle formation (4 hours),

Composition of inorganic and organic particles- toxic metals and radioactive particles Effects and control of particles (4 hours)

Unit 2. Water Pollution: Water quality - Water pollutants (inorganic and organic) - Sources, fate (3 hours),

Effects and controlling measures - Chemical speciation, Pollution by Radionuclides (3 hours),

Biochemical oxygen demand-Chemical oxygen demand (3 hours), Eutrophication, Biodegradation of pollutants (3 hours).

Unit 3. Water treatment

Hardness of water and its removal - removal of solids and other toxic materials, Treatment of water for drinking (2 hours)

Electrodialysis, ion exchange, Reverse osmosis, desalination processes, Removal of iron, manganese, phosphorous, calcium and nitrogen (2 hours),

Treatment of water for industrial purposes, Sedimentation, coagulation, flocculation, filtration, Adsorption, disinfection of water, Sewage treatment (physical and chemical methods), Health effects of drinking water treatment technologies (2 hours),

Impact of detergents, pesticides and other additives on sewage treatment, Oils in Fresh & Marine Water: Sources of oil pollution -Chemistry and fate of hydrocarbons, Oil in run off and ground water, Biodegradation effect on aquatic organisms, Treatment and disposal technology (2 hours)

Unit 4. Soil Pollution

Soil pollutants -Inorganic, organic, Pesticides, radionuclides, (2 hours)

Sources and effects on nature and properties of soil, crops, plants and terrestrial animals (2 hours).

Unit 5. Hazardous Wastes and Values in Environment

Nature and sources of hazardous wastes, Classification, characteristics & constituents (2 hours),

Transport and effects, Hazardous wastes in Geosphere (2 hours),

Hydrosphere, Biosphere and Atmosphere (2 hours),

Reduction, treatment by physical and chemical methods (2 hours),

Thermal treatment methods, Biodegradation of wastes, Disposal of hazardous wastes (2 hours).

Waste management and Industrial by-products, Natural hazards and management- control of subsurface migration of Hazardous Waste (2 hours),

E-Waste: effect on environment: Sources-constituents and their effects-pollution of water, soil and air-Methods of treatment and disposal-Extraction of gold and other precious metals from E-waste (2 hours)

Values in Environment: The philosophy and Technology of living in tune with nature and its assets, Nature-A silent teacher, Ecology-The Indian Approach. (2 hours)

Prescribed Books:

- (1) Stanley E. Manahan, Environmental Chemistry .10th Ed., CRC press, 2017.
- (2) B.J. Finlayson– Pitts and N.N. Pitts Jr., Atmospheric Chemistry, Wiley, 2000.

Reference Books:

- (1) A.K. De, Environmental Chemistry, 2nd Ed., Wiley Eastern, 2016.
- (2) R.M. Harrison Pollution: Causes, Effects and Control, 3rd Ed., Royal Society of Chemistry, London, 2001.

| Course category | Course Code | Course Name | L | T | P | C |
|--------------------------------|--|-------------------|---|---|----|---|
| DSE | MCHR2248 | Project II | - | - | 16 | 8 |
| Course Learning Outcome | | | | | | |
| CLO1 | To plan and carry out research using various analytical tools/methods. | | | | | |
| CLO2 | To analyse the results using various tools | | | | | |
| CLO3 | To write an article and present the findings to the scientific community | | | | | |

Project II is the continuation of project I. Proposal presented in project I (SEM III) is to be carried out under the guidance of internal faculty member in this semester. Students going for internship are required to fulfil the same. The evaluation would be done at the end of the semester. Head of the department constitutes the committee for the purpose. Students would be required to present his/her research findings to a committee constituted by the Head of the department.